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Optimization of Materials Microstructures: Information Theory Approach

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Abstract

The effect of heterogeneity and microstructure of materials on their fracture resistance is analyzed with the use of the information theory approach. Interrelations between the microstructure and heterogeneity of materials, the crack path structure and fracture resistance are studied analytically, and then compared with the literature data. It is shown that the maximum information entropy of distributions of local parameters of weaker phases (like orientations, spatial distribution, local properties) in materials ensures higher fracture resistance. An increase of the entropy of distributions of local parameters of weaker phases (and, therefore, the increase of the fracture toughness) can be achieved both through increased scattering of the parameters and by using hierarchical microstructures.

1. Introduction

It has been shown in many works (see e.g. [1-3]), that, along with the chemical and microscopical methods of improving mechanical properties, there exists the mesoscopical way to increase the strength of materials: namely, the mechanical properties of materials can be improved by varying distribution and arrangement of phases in two-phase materials, without changing the properties of phases. The purpose of the paper is to analyze the effect of heterogeneity of materials on their fracture resistance and possibilities to improve the materials microstructure. The interrelations between the microstructure and heterogeneity of materials, the crack path structure and fracture resistance are considered on simple examples, and then compared with the literature data on the materials optimization.

As a measure of the heterogeneity, the Shannon’s information of distribution of local parameters of materials is used [3, 4]. This value is taken here since it characterizes not only the scattering of local parameters, but it has also a deep meaning, as a characteristics of the degree of ordering in complex systems [3, 5]. The meaning of the "information" as a characteristic of the material microstructure may be formulated as follows. When a material is formed, some information is fixed in it in the form of the heterogeneity of different local parameters (distributions of phases and inclusions, their sizes, etc). When the material is loaded and fail, this heterogeneity (information) determines the way and patterns of the material behaviour during destruction. When cracks grow, the heterogeneity of the material increases. Therefore, the chain "conditions of the formation of the material - > its behaviour under loading -> deformation and failure patterns" can be considered as an information transformation system.

In order to compare the performances (strength or fracture resistance) of materials with different microstructures, a general criterium of the closeness of the material to failure is required. Here, the closeness of a specimen to failure is characterized by the "fuzzy damage parameter", suggested in [3, 6].

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This parameter is defined as the ratio of a current value of some strength characteristics of the material (like K_I or loading time) to the critical value of this parameter (like K_{Ic} or time-to-failure at a given load):

$$D = K_I/K_{Ic}, \text{ or } D = t/t_{cr}, \qquad (1)$$

where K_I - stress intensity factor, K_{Ic} - critical stress intensity factor, t - loading time (at static loading), t_{cr} - time-to-failure at a given load [3, 6, 7].

2. Heterogeneity of Materials, Crack Path Structure and Fracture Resistance of Materials: Some Examples

In this section, we consider several very simple qualitative examples which should demonstrate the relationships between statistical parameters of the crack path, microstructure of material and the fracture resistance of the material. We use here the following approach: a simple model of crack propagation is taken; then we look at the probability distribution of local parameters of fracture (as variations of crack direction, sites of crack initiation, crack sizes, etc.) and determines the informational entropies of the probability distribution for two extreme cases: homogeneous material (i.e., classical fracture mechanics case) and randomly heterogeneous material. By comparing the fuzzy damage parameter D for these two cases, we try to make some conclusions about the interrelations between the heterogeneity (entropy) of the material and its strength.

2.1. Variations of Crack Path

Consider now a simple model of crack propagation. A crack grows in a discrete lattice, and may increase by a unit step either in vertical or in horizontal direction (see Figure 1). The load is applied in vertical direction.

Let us look at variations of the directions of unit steps of crack growth. If p_1 is the probability that the next unit step of crack growth is horizontal, and p_2 that it is vertical, the informational entropy of the probability distribution of the step orientation H is given by the formula:

$$H = - p_1 \ln p_1 – p_2 \ln p_2, \qquad (2)$$

where p_2=1 – p_1. In the case of a homogeneous material, crack grows straightforward, p_1 =1 and p_2=0. In a heterogeneous material, the strength distribution of lattice units has a random component. Then, p_2 >0 due to the randomness of the strengths of local units. Yet, p_2 still can not be greater than p_1 (a crack can hardly grow in the direction parallel to the applied tensile force). The value H is maximal, when p_1 = p_2 [4]. So, the more disordered is the material, the greater is p_2 and the greater is H. The nominal crack length L (the distance between the ends of the crack) can be determined as

$$L = p_1 \Delta L\, N, \qquad (3)$$

where ΔL – unit step of the crack growth, N – general amount of the steps of the crack growth.

If one characterizes the closeness of the specimen to failure (“fuzzy damage parameter”, see [6]) in the simple form as

$$D = K_I/K_{Ic}, \qquad (4)$$

and taking into account the interrelations between L and p_1, one may obtain

$$D \sim \sqrt{p_1 \Delta L N} \; / \; K_{Ic} \qquad (5)$$

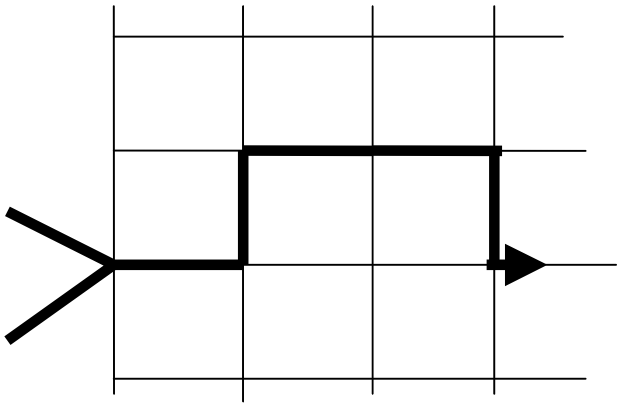


Figure 1. Crack growth in a lattice with randomized properties (scheme).

Therefore, one can see that the smaller is the value H the closer is the specimen to failure (all other conditions the same). One may speculate also, which microstructures of material can ensure high p_1 and high H: evidently, layers of a weak material oriented perpendicular to the expected crack growth direction increase the value p_1, and therefore H and the fracture resistance of such a material. Such layers may present fibers, or weak fiber/matrix interface, or brittle inclusions, like primary carbides in high speed steels.

2.2. Distribution of sites of crack initiation

Let us look now at the effect of the spatial distribution of crack initiation sites on the fracture resistance of the material. Take a volume with a cut, which consists on K unit cells. Each of the cells can fail (analogue of the crack initiation) or stand. If the material is homogeneous and the volume is loaded as shown in Figure 2, the probability of failure of the cell A is equal to 1, and the entropy of the probability distribution of failure over the cells is

$$H = - \Sigma_K \, p(i) \ln p(i) = - p(A) \ln p(A) = 0, \qquad (6)$$

where p(i) - probability of failure in the i-th cell, i = 1...K. If the material is non-homogeneous, $p(A)<1$, and $H>0$. Thus, the greater is the probability of failure of the cell B, the greater is the entropy H. In the first case [homogeneous material, p(A) =1 and p(B)=0],

$$D_1 \sim \sqrt{L_0 + \Delta L} \, / \, \sqrt{L_{cr}} \qquad (7)$$

where L_0 - initial notch length, ΔL - cell size, L_{cr} - critical length of a crack. In the second case [a material with weak regions], $p(B)>0$ and $p(A)<1$. If $p(A) <1$, D_2 becomes statistically less than D_1. Therefore, one can see the correlation again: the greater is the in the material, the stronger is the material. Practically, a microstructure has a high statistical entropy of the local failure probability over the sites, if some phases and inclusions in the materials at some distance from the notch tip are much weaker than the material at the notch tip and can therefore present competing sites of the microcrack initiation. It is clear that an increase in the entropy of the sites of crack initiation (practically, it means an increase of amount of crack nuclei in the material under loading) leads to the increasing of the entropy of the crack size distribution as well.

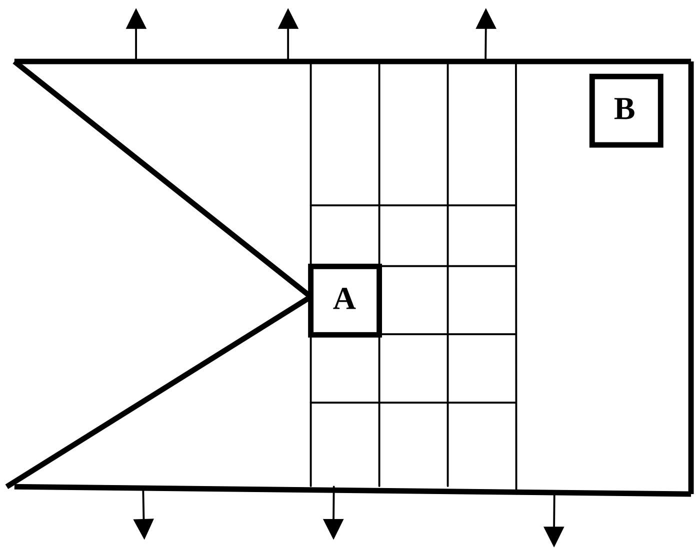


Figure 2. Initiation of microcracks in front of a growing crack (cell A) and in a random site (cell B) (scheme).

2.3. Variations of local properties of the materials

Consider now two cases shown in Figure 3. The loaded material is supposed to be homogeneous and consists on the phase X in the first case (Figure 3a), and randomly heterogeneous and consist on the phases Y and Z in the second case (Figure3b). The average strength of the material is the same in both cases, yet, the phase Y is (1+c) times stronger and the phase Z is (1-c) times weaker than the phase X. The elastic properties of both phases supposed to be the same. The criteria of local failure of the phases X, Y or Z is the critical level of von Mises stress: $\sigma=\sigma_{cr}$. The crack is supposed to grow straightforward. The expected crack path is presented as a number of cells [1].

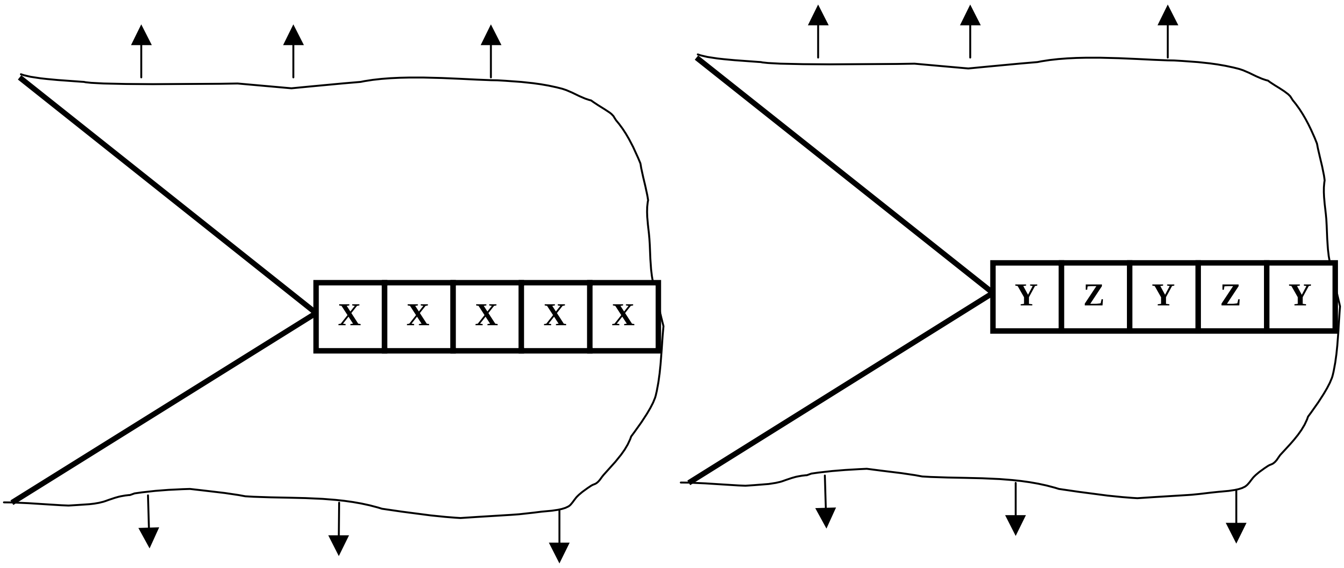
The energy consumption for crack growth is:

$$G = mA/lbm = A/lb, \qquad (8)$$

where A - energy of failure of a unit cell (Figure 3), l - cell size, b - width of the 2D problem, m - amount of the cells per unit length. The energy is proportional to σ_{cr}^2: A ~ $\sigma_{cr}^2/2E$, where E - Young modulus of the material. For the first case (a homogeneous material X; Figure 3a): $G_1 \sim m\sigma_{cr}^2/2lbE$, and for the second case:

$$G_2 \sim [p_Y (1+c)2\sigma_{cr}^2 + p_Z (1-c)2\sigma_{cr}^2]/2Elb \sim [1+c^2 + 2(p_Y-p_Z)c]\, G_1, \qquad (9)$$

where p_Y and p_Z= 1-p_Y - volume contents of phases Y and Z in the second case. In the simplest case, when p_Y=p_Z, G_2/G_1 ~ 1+c^2. Let us look now at the entropies of the phase properties: in the first case, H_1 = 0, and in the second case, H_2 =- p_Y ln p_Y - p_Z ln p_Z = 0.69. Thus one can see that an increase in the heterogeneity of the local properties of the material (the averaged values the same) leads to the increase of the fracture resistance of the material.



a) b)

Figure 3. Crack growth in a homogeneous material (a((phase X) and in a heterogeneous materials (b), phases Y and Z (scheme).

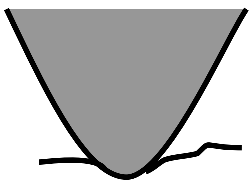
2.4. Contact problem and wear

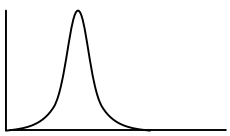
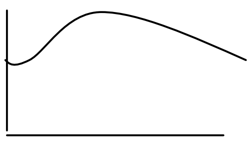
One may note that in all three cases considered above the strength of material increases if the heterogeneity of local parameters of crack path increases. It is of interest to compare this conclusion with the results from [3, 8]. In [8] it was shown that the efficiency of a destructing tool increases if the informational entropies of "distributed parameters of the tool" increase. Among the "distributed parameters of a tool", the contact stress (for increasing of the sharpness of tool), wear-resistance in a point of tool work surface (durability of tool, the self-sharpening of tool and high efficiency of drilling tool even after a lapse of time of drilling), orientation of destructing elements (teeth) and distances between them on the tool, rate, direction and mechanism of loading by each element of complex tool are listed.

It was shown in [8] also, that the long-term efficiency of the tool can be achieved if the information entropy of the distribution of local wear-resistances of the tool work surface is high enough. Practically, it means that in order to ensure the high efficiency of material fragmentation by a destructing tool during long time, the tool working surface should consist on a number of components with different wear-resistances. This analysis allowed to formulate a general principle of improvement of destructing tool (the greater are the informational entropies of local parameters, the better is the efficiency of the tool). Table 1 gives the main ideas of the informational approach to the tool design in a compact form.

Comparing the conclusions from the sections 2.1-2.3 and [8], one may draw a conclusion that by increasing initial scattering of the local strength, orientations and spatial distribution of constituents of interacting bodies, the performances of a material, a specimen or a tool may be improved for longer time period.

Table 1. Main points of the informational approach to the tool improvement [8]

<table>
<tr><td colspan="3">Main Ideas:</td></tr>
<tr><td></td><td colspan="2">$P(\sigma)=N[\sigma]/N$,
where σ - contact stress, P(σ) - probability of a given stress σ, N[σ] - amount of contact points in which the stress is equal to σ, N - total amount of contact points between the indenter and the material.

$H = -\Sigma P(\sigma) \log P(\sigma)$,
- entropy of the probability distribution P(σ).</td></tr>
<tr><td colspan="3">Examples:</td></tr>
<tr><td>Type of the probability distribution</td><td>Value H</td><td>Meaning</td></tr>
<tr><td>P(σ)  σ</td><td>low</td><td>Only one level of stress is probable; stress distribution is homogeneous.</td></tr>
<tr><td>P(σ)  σ</td><td>high</td><td>Many levels of stress are probable; high stress concentration.</td></tr>
</table>

3. Optimization of Materials: Some Literature Data

Consider literature data about the methods of the improvement of fracture resistance of materials. The results collected from different sources are given in Table 2. One may note that the recommendations given in the table are related mostly to different materials; yet, the common tendencies in the material development may be observed.

It is of interest to compare the conclusions given in the Table 2 with the above analytical conclusions. We shall use the following designations in the references to the Table: "A2" means the second recommendations given by the author A... or by the author A... et al.

One can see that the recommendations R1, M1, M2, T2, T3 and G1 correspond to the principle formulated in the section 2.1: the increasing of the entropy of orientation of directions of crack steps increases the fracture resistance of the material. This can be achieved by crack deflection on the layers of weak inclusions perpendicular to the expected crack growth direction (M1), or a network which sets the crack path (R1), or a network from layers of brittle/weak inclusions (G1, M2), or by "fluctuated residual stress" from nano-particles which causes "zigzag crack path " (T2).

The recommendations E1 and M3 correspond to the principle formulated in the section 2.2: the availability of many sites of potential crack initiation (instead of one single weak place in the specimen) increases the fracture resistance. This is achieved by the availability of weak elements (brittle second phase particles) which fail when the material is loaded and consume the energy of crack growth. The recommendation W2 corresponds to the principle given in the section 2.3: adding the heterogeneity in a material increases its fracture resistance.

Table 2. Some recommendations on the improvement of fracture resistance of materials [1]

Authors	**Materials considered**	**Ways to increase fracture resistance of materials**	**Designa-tions**
Evans et al [9] and Evans [10]	high temperature engineering ceramics and ceramic matrix composites	1. Controlled microfracture (i.e. the material contains brittle second phase particles which fail in the stress field of a growing macrocrack and therefore increase the energy consumption in the crack propagation). This approach does not lead to the increase of fracture strength. 2. Ductile second phase network. "Cylinder" particles of ductile second phase (practically, it can be realized as continuous network of ductile phase along grain boundary triple points) are better reinforcement than the spherical second phase particles. 3. Frictional toughening (which is achieved in materials containing strong aligned reinforcements with weak interfaces, which enable debonding and allow dissipation by internal friction). This mechanism is more effective than ductile phase toughening (which is achieved by ductile reinforcement in an elastic matrix).	E1-E3
Raj and Thompson [11]	Ni/Al2O3, Pb/ MgAl2O4, WC/Co and other composites	It was shown that fracture toughness of MMC with continuous network from precipitates (like WC-Co, Al-Al, produced by liquid phase sintering or Lanxide process) is much higher than that for dispersed particles (fabricated by hot pressing of powder mixtures of metal and oxide followed by reduction of oxide into metal).	R1
Watanabe and Kawasaki [12]	functionally gradient metal-ceramic sintered (also hot pressed and HIP) composites	1. Increasing the connectivity of the metal phase (Betty number) leads to the increase of fracture toughness 2. Crack arrest function of FGM is improved by metal fiber premixing in the ceramic-rich region.	W1-W2
Mishna-evsky Jr et al [13, 14]	high speed steels (HSS)	Effects which increase the fracture toughness of the steels: 1. crack deflection by the carbide layers oriented perpendicularly to the initial crack path (observed in the net-like coarse microstructure, band-like microstructures), 2. the crack follows the carbide network (net-like fine microstructure), and 3. damage formation at random sites of the steels and following crack branching (random microstructures). Fracture resistance of steels increases generally in the following order: band-like -> random -> net-like microstructure.	M1-M3
Tan and Yang [15]	nano-composite alumina ceramics with dispersed Si nano particles	Higher toughness of nano-composite ceramics is shown to be achieved by particles distributed within the matrix grains along grain boundaries. Three toughening mechanisms were identified: 1. "switching from the intergranular cracking to the transgranular one" (by nano-particles distributed along the grain boundaries), 2. "fracture surface roughening by zigzag crack path" (by the	T1-T3

		fluctuated residual stresses from the nano-particles within the grains), and 3. "shielding by clinched rough surfaces near the crack tip".	
Gross-Weege et al [17] and Berns et al [16]	Ledeburitic chromium steels	Fracture toughness of steels can be increased by 1. increasing the width of crack path (in the hardened and low tempered states) (this is achieved by increasing the cell size in netlike structure of steels, or by using netlike structure instead of band-like structure of steels) ; 2. increasing the part of crack path through ductile matrix (in the soft annealed states) (is achieved by increasing the matrix ductility, for instance, by increase in the temperature of tempering).	G1-G2
Berns et al [18]	Ledeburitic chromium steels	"Double dispersion" microstructure of the steels (i.e. the coarse hard phase - primary carbides- is replaced by a dense dispersion of small carbides) ensures sufficiently higher fracture toughness and lifetime.	B1

4. Some Ideas on the Materials Optimization

As can be seen from Table 2, among the main ways of increasing the fracture resistance of multiphase materials the following approaches may be mentioned: adding second phase particles or network, which cause accompanying, energy-consuming processes during crack growth in the first phase (matrix) (like friction, additional microcracking, etc.); varying degrees of phase networking and clustering; creating such an arrangement of inclusions that a growing crack deflects most frequently from the path which it would follow in a homogeneous material (like the pure matrix) (this is achieved by ductile inclusions, like metal fiber premixing in the ceramic-rich region [12], or weak interfaces [9] , or special arrangements of brittle inclusions);

In the section 2 it was shown that the increase of fracture resistance can be achieved if the informational entropies of probability distributions of different local parameters of fracture (as sites of crack initiation, directions of crack propagation, etc.) increase. This can be done through the corresponding increase of the entropy of the distribution of weak elements/phases in the material. Thus, one may formulate the following principle: the **increased scattering** (i.e., information entropy of probability distributions) **of local parameters of weaker phases** in the material ensures higher fracture resistance.

The new material developed by Berns et al [18] ("double dispersion structure") is especially interesting for our analysis. The "double dispersion structure" presents an hierarchical microstructure: instead of large carbides, the steel contains areas of high concentration of small carbides. From the entropy additivity principle [4] follows that the entropy of a system which includes subsystems presents a sum of the entropy of the subsystem and the macrosystem. Therefore, taking into account the above interrelations between the entropy parameters and strength, one may expect that hierarchical material structures ensure higher strength than simple microstructures. The results by Berns et al. [18] confirm this conclusion. This suggests to consider another way to improve the material strength by varying the entropy parameters, namely **hierarchical distribution** of weaker phases in materials. Probably, this can be efficient not only in the case of "double random" microstructures (like in the case of [18]), but also for "double network" or "double layered" or mixed microstructures.

The stability and reliability of complex information systems may be improved by including feedbacks in the system [4]. This possibility in this case is given by using the interrelations between phase transitions in loaded solids and the strain state. Steels with high ductility and tensile strength can be developed using the transformation induced plasticity (TRIP) phenomena which accompanies the martensitic phase change in ductile materials [19, 20]. So, the self-organization of materials [21, 22] can be achieved by combining required distributions of phases (especially, weaker phases) and the feedbacks mechanisms.

5. **Conclusion**

The effect of variations of local properties of materials on their fracture resistance was studied analytically. It was shown that the maximum information entropy of distributions of local parameters of weaker phases (like orientations, spatial distribution, local properties) in the material ensures higher fracture resistance. The increase of the entropy (and, consequently, the increase in the fracture resistance) can be achieved both through increased scattering of the parameters and by using hierarchical microstructures. The possible ways of improving materials microstructures on the basis of this approach are discussed.

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