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Nucleation and Growth of Microcracks: an Improved Dislocational Model and Implications for Ductile/Brittle Behaviour Analysis

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ABSTRACT Presented is an analysis of the early stage of the fracture process in a crystalline solid – the nucleation and development of dislocational cracks. For description of the fracture precursors' evolution, the improved discrete-continuum model of Stroh-type dislocational pile-up has been worked out. The investigation of peculiarities of dislocations interaction at short distances in the stress field showed that microcrack nucleation and growth result from the equilibrium stability loss at the pile-up head and further joining of leading dislocations there. The criteria of microcrack nucleation and growth are derived accounting for the role of both shear and tensile stresses. On this basis the macrocriterion of fracture at a point of an elasto-plastic solid was derived in terms of values of plastic strain, maximum normal, and shear stresses which comprise some microstructural characteristics of the material. Discussed is the transition from the stress-controlled fracture to the strain-controlled one, as well as the prerequisites of ductile (brittle) behaviour depending on the stress state triaxiality and material microstructural peculiarities.

Introduction

Plastic strain in crystalline solids at a moderate temperature is a prerequisite of any fracture, including a brittle one. This was suggested first by Stepanov **(1)**, and later experimentally confirmed and theoretically developed in numerous works in the field of physics of materials strength. The dislocational nature of the process of (micro)plastic deformation-and-fracture has been proved. It was found, e.g., **(2)**, that formation and behaviour of the groups of the same-sign excess dislocations – dislocational pile-ups – determine nucleation and development of microfractures – dislocational cracks. Before being completed the process may pass through a number of subsequent stages: formation of blunt structural cracks, formation of pores, etc. **(2)**. Depending on the length of the chain of stages required for fracture completion under the given conditions, it will be more brittle or ductile. In this case continuation (completion) of a rupture to a great degree depends on conditions providing accomplishment of the initial event – dislocational crack formation. For their analysis, the

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improved microfracture model is developed; it describes both nucleation and growth of microcracks within a unique framework. The criteria of microcrack nucleation and spreading are obtained here naturally, i.e., without any additional condition, from only the analysis of the pile-up equilibrium stability in the stress field.

Model of dislocational crack nucleation and growth

The model described below is the result of combining the two approaches of the physics of fracture developed earlier: discrete-continuum modelling of dislocational pile-ups and models of atomistic cohesive forces for the description of defects in solids **(3)–(5)**.

Dislocational pile-up model

Considered is a pile-up of n edge dislocations with Burgers vector $\boldsymbol{b}$ (Fig. 1). Stresses in the pile-up vicinity, both shear $\tau_{xy} = \tau_t$ and normal to the plane of the expected cleavage $\sigma_{xx} = \sigma_n$ are determined by the solid macroscopic stress field. Stress τ_t pushes the pile-up to the obstacle located in the plane $x = 0$.

In this pile-up with the total Burgers vector $\boldsymbol{B} = n\boldsymbol{b}$, its leading element B_1 and dislocation B_2 following it are singled out and described individually, while the remainder part of the pile-up $B_3 = \boldsymbol{B} - B_1 - B_2$ is considered to be continuous. The cores of elements B_1 and B_2 are supposed to be wedge-like cavities with interacting faces in the elastic continuum similarly to the

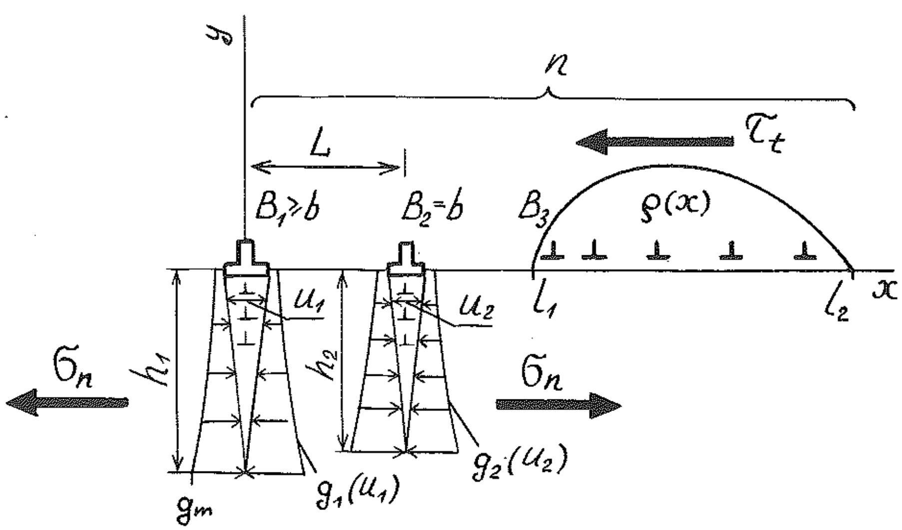

Fig 1 Model of blocked flat pile-up of edge dislocations

accounting for cohesive forces in the crack tip zones **(3)**. The cores are considered to be the distributions of infinitesimal 'cleavage' dislocations with densities $\eta_j(y)$ on sections $[-h_j, 0]$ (Fig. 1), for which $\int_{-h_j}^{0}\eta_j(y)\,dy = B_j$ $(j = 1, 2)$. The opposite faces of the core of any of the elements B_j are attracted by the forces of inter-plane cohesion in the crystal $g_j(u_j)$, where the core opening $u_j(y) = \int_{-h_j}^{y}\eta_j(y)\,dy$. The part B_3 occupying the interval $[l_1, l_2]$ of axis $0x$ is described by the density $\rho(x)$ of gliding edge dislocations, and $\int_{l_1}^{l_2}\rho(x)\,dx = B_3$.

The equilibrium equations of such dislocational formation comprise (i) equilibrium equations of cores of elements B_j under stresses $\sigma_{xx}(x, y)|_{x=L_j} = \sigma_n + \sigma_{xx}(B_k) + \sigma_{xx}(B_3)$ $(j, k = 1, 2; j \neq k$; $L_1 = 0$ and $L_2 = L$ are coordinates of elements B_1 and B_2; $\sigma_{xx}(B_{j'})$ are the stresses produced by elements $B_{j'}$ of the pile-up, $j' = 1, 2, 3)$; (ii) equilibrium equation of part B_3 under stress $\tau_{xy}(x, 0) = \tau_t + \tau_{xy}(B_1) + \tau_{xy}(B_2)$; (iii) balance condition for the forces acting in the slip plane on movable dislocation B_2, i.e., as a result

$$M\left[\int_{-h_j}^{0}\frac{\eta_j(\xi)}{\xi - y}\,d\xi + \int_{-h_k}^{0}\eta_k(\xi)\,\frac{(\xi - y)\{3L^2 + (\xi - y)^2\}}{\{L^2 + (\xi - y)^2\}^2}\,d\xi - \int_{l_1}^{l_2}\rho(\xi)\,\frac{y\{3(L_j - \xi)^2 + y^2\}}{\{(L_j - \xi)^2 + y^2\}^2}\,d\xi\right] = g_j(u_j) - \sigma_n \quad (j, k = 1, 2; j \neq k) \tag{1}$$

$$M\left[\int_{l_1}^{l_2}\frac{\rho(\xi)}{\xi - x}\,d\xi - \sum_{j=1,2}\int_{-h_j}^{0}\eta_j(\xi)\,\frac{(x - L_j)\{(x - L_j)^2 - \xi^2\}}{\{(x - L_j)^2 + \xi^2\}^2}\,d\xi\right] = \tau_i - \tau_t$$

$$F_{B_1B_2} + F_{B_3B_2} - B_2(\tau_t - \tau_i) = 0 \quad \left(M = \frac{E}{4\pi(1 - \mu^2)}\right)$$

where τ_i is the lattice friction stress, E is the Young modulus, μ is the Poisson ratio, forces $F_{B_jB_2}$ of elements B_2 and B_j interaction $(j = 1, 3)$ are

$$F_{B_1B_2} = ML\int_{-h_1}^{0}\eta_1(y)\int_{-h_2}^{0}\eta_2(\xi)\,\frac{L^2 - (\xi - y)^2}{\{L^2 + (\xi - y)^2\}^2}\,d\xi\,dy, \tag{2}$$

$$F_{B_3B_2} = M\int_{l_1}^{l_2}\rho(x)\int_{-h_2}^{0}\eta_2(y)\,\frac{(L - x)\{(L - x)^2 - y^2\}}{\{(L - x)^2 + y^2\}^2}\,dy\,dx. \tag{3}$$

In order to analyse the fracture nucleation and development, the mathematical model of equations (1)–(3) should be completed by the condition for limit equilibrium of the pile-up head part. Two ways of the pile-up transfer into the instability are possible: (I) loss of equilibrium stability of the crack-like core of element B_1, i.e. its progressing opening in the cleavage plane as the Griffith type crack under the action of stress $\sigma_{xx}(0, y)$, which will occur when

$$h_1(B_1, \sigma_{xx}, g_1) \geqslant h_c \quad (\sigma_{xx} = \sigma_n + \sigma_{xx}(B_2) + \sigma_{xx}(B_3)) \tag{4}$$

where h_c is the critical size of B_1 core; (II) instability of dislocation B_2 position, its dropping to B_1 and their joining leading to the spreading of the wedge-like dislocational crack which takes place when the condition is satisifed

$$\partial F_{B_2}/\partial L = 0 \qquad (5)$$

where F_{B_2} is the total force acting upon the dislocation B_2 in the glide plane.

The critical combination of the governing parameters of dislocational pile-up n, τ_t, σ_n, corresponding to the microcrack nucleation or propagation at its head, are determined by the less severe conditions of equations (4) or (5).

The solution of equation (1) in the explicit form is accessible only by numerical methods in which the obtaining of general conclusions is difficult. But when $B_1 + B_2 \ll B$, and, hence, $L < l_1 \ll l_2$, the analysis is simplified and the desired result may be obtained approximately in the closed form **(6)**. In this case when considering the structure of each element B_k ($k = 1, 2, 3$) of the pile-up, the action of elements B_j ($j \neq k$, $j = 1, 2$) is accounted for in the approximation of the long-range elastic field, i.e., it is accepted that $\eta_j(y) = B_j\,\delta(y)$ where $\delta(y)$ is the Dirac delta-function. Then the first three equations of the equation system (1) become independent singular integral equations. Their solution by the generally known Muskhelishvili method results in functions which determine the configurations of the leading elements B_1 and B_2 (6)

$$\eta_j(y) = \frac{1}{\pi M\sqrt{\{-y(y+h_j)\}}}\left\{(S_k + S_3)\left(y^2 + \frac{h_j}{2}y - \frac{h_j^2}{8}\right)\right.$$
$$- \sigma_n(y + h_j/2) + B_j M - \frac{1}{\pi}\int_{-h_j}^{0}\frac{\sqrt{\{-\xi(\xi+h_j)\}}}{\xi - y}\,g_j\{u_j(\xi)\}$$
$$\left. + 0(h_j^2/L^2)\right\} \quad (j, k = 1, 2;\ j \neq k) \qquad (6)$$

where values $S_k = 3B_k M/L^2$, $S_3 = 3M(B_1 + B_2)/(8l_1^2)$ reflect the effect of normal stresses $\sigma_x(B_k)$ and $\sigma_{xx}(B_3)$ upon the structure of element B_j.

Microcrack nucleation

At this stage of the process both leading elements of the pile-up are still the ordinary lattice dislocations, i.e., $B_1 = B_2 = b$. The structure of their cores is determined by the identical densities of the cleavage dislocations, due to which the indices in designations of densities $\eta(y)$, lengths of cores h, etc., are omitted here.

The following approach, used before in analysing the cracks **(3)**, continues the parallelism inherent to the description of dislocations and cracks **(4)(5)**. The non-linear law of the interplane cohesion in the crystal is replaced by the 'force–displacement' dependence with the initial linear part reaching the maximum g_m of the real interaction curve, i.e., the theoretical strength in the given cleavage plane, while the interaction corresponding to the cohesive forces diminishing in the core region $-h \leqslant y \leqslant 0$ is specified in parametric form by the linear relation (for the scales of atomistic sizes it ought not to be looked for the physical grounds) $g\{u(y)\} = g_0 + (g_m - g_0)y/h$, where the core characteristic $g_0 = g(u)|_{y=0}$ may be found, for example, from the data on the energy of the core of given crystallography.

Now equation (6) completely determines the structure of the dislocation cores in the stress field inherent to the region of the pile-up head. The core size is found from the condition of the finiteness of stresses at their ends $y = -h$, which is equivalent, as it is known **(3)**, to the condition $\eta(-h) = 0$, from which via equation (6) we obtain

$$h = \frac{1 - \sqrt{\{1 - 3h_0^2(S_2 + S_3)/(2bM\}}}{3h_0(S_2 + S_3)/(4bM)} \qquad (7)$$

where $h_0 = 2bM/\{3g_m/4) + (g_0/4) - \sigma_n\}$ is the core size with the pile-up absent. The latter agrees with the known evaluations of the more adequate microscopic models **(2)(7)**.

Equation (7) shows that under the action of stresses caused by the pile-up the size of the cores of its leading dislocations h may grow up to the limit value $h_c = 2h_0$. At $3h_0^2(S_2 + S_3)/(2bM) > 1$ there are no real values of the equilibrium size h, which means the instability of the dislocation core and its transformation into the spreading crack (type I instability). The condition of equation (4) takes the form

$$h \geqslant 2h_0 \quad \text{or} \quad 3h_0^2(S_2 + S_3)/(2bM) \geqslant 1 \qquad (8)$$

and up to its fulfilment $h/L \leqslant h_c/L_c = \sqrt{[8\{1 - 3h_0^2 S_3/(2bM)\}]/3} < 1$, where L_c determines the position of dislocation B_2 when reaching the type I instability.

To determine the condition of the type II instability let us consider the interaction of dislocations B_1 and B_2. For the alternative to the condition of equation (8), we shall deal later only with the region $L > h_c$, i.e., $h < h_c$ and $h/L < 1$.

Using equations (2) and (6) we obtain

$$F_{B_1B_2} = \frac{Mb^2}{L}\left[1 - \frac{\chi(\zeta)}{\zeta^2}\right] + 0(\zeta^{-5}), \qquad (9)$$

where $\zeta = L/h_c > 1$, $\chi(\zeta) = [h(\zeta)/h_c]^2$. This result agrees with the lattice **(7)** and 'quasi-atomistic' **(4)** physical models.

Here important is the fact that the force of dislocation interaction comprises the component of mutual attraction caused by the interaction of their cores. This component becomes essential at short distances between them. Its presence allows for the possibility of positional instability of dislocation B_2 at the pile-up head.

From equation (9) it can be determined that in the region considered, $\zeta \geqslant \zeta_c = L_c/h_c$, the force $F_{B_1B_2}(\zeta)$ reaches the maximum $F_{B_1B_2}^{\max}$ at $\zeta = \zeta_m = L_m/h_c$, and then at $\zeta \gg \zeta_c$ it changes as $\zeta^{-1} \propto L^{-1}$ (Fig. 2). The behaviour of $F_{B_1B_2}(\zeta)$ depends on the parameter $A = 3h_0^2 S_3/(2bM)$, i.e., on the pile-up capacity and

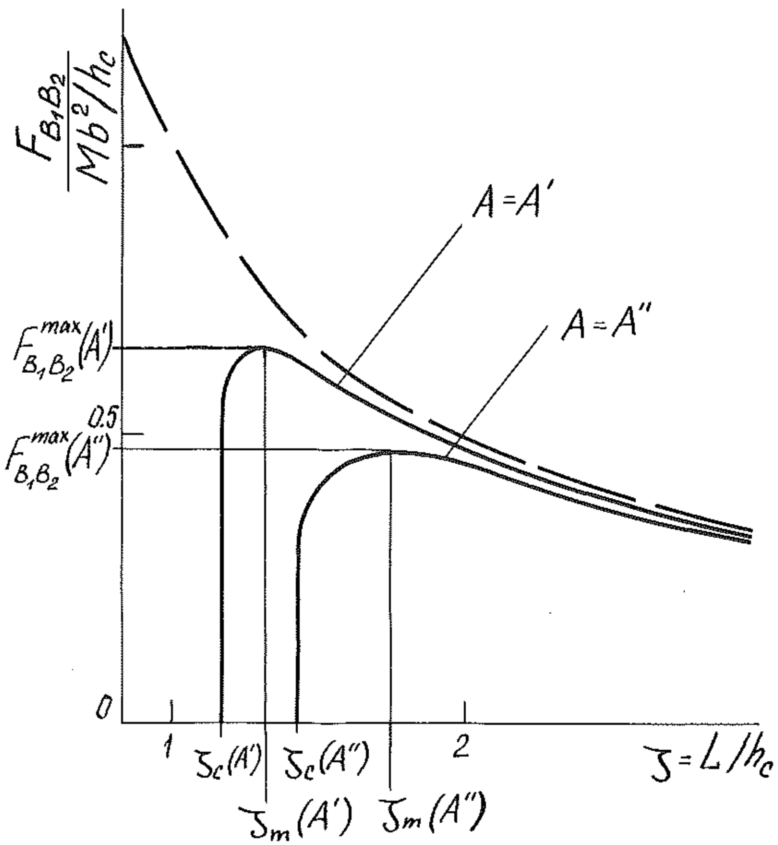

Fig 2 Interaction (repulsive) force of pile-up leading elements B_1 and B_2 separated by distance L: broken line – the known dependence of the continuum dislocations theory of type $F_{B_1B_2} = MB_1B_2/L$; solid lines – result of equation (9) which accounts for the interaction of dislocation cores depending on external stresses and those produced by the remainder part of pile-up ($A = A\{\sigma_n, \sigma_{xx}(B_3, \tau_t)\}$, $A' < A''$)

external stresses. Solution of the equation $\partial F_{B_1B_2}/\partial\zeta = 0$ gives **(6)**

$$\zeta_m = \zeta_c\left\{1 + \frac{32(1-A)^3}{(24A^2 - 36A + 21)^2}\right\}, \quad \zeta_c = \frac{3}{\sqrt{\{8(1-A)\}}} \tag{10}$$

$$F^{\max}_{B_1B_2} = F_{B_1B_2}(\zeta_m) = \frac{Mb^2}{h_0}\frac{\sqrt{\{2(1-A)\}}}{27}\left\{5 + 4A + \frac{32(1-A)^3}{24A^2 - 36A + 21}\right\}. \tag{11}$$

The result of equation (11) is very close to the one **(4)** obtained for the case of $n = 2$ and $\sigma = 0$ with the physically more exact model of the core. This means that the model of the cohesive forces is a sufficiently good approximation for description of the dislocation cores.

The critical combination of the parameters n, τ_t and σ_n, corresponding to the breakdown of the B_2 dislocation position stability, is determined from the equations system formed by the latter equation from equation (1) together with equation (5). The analysis showed **(6)** that with a small error, the solution of equation (5), i.e., the position of the B_2 dislocation unstable equilibrium, is determined by the value $L = L_m$ (or $\zeta = \zeta_m$). When the pile-up leading dislocations are pushed together by such a distance, the dislocation B_2 falls to B_1 and the formation of a superdislocation with Burgers vector $2b$ occurs. At least for the BCC metals **(2)** the core of such a dislocation forms a cavity with non-interacting faces, i.e., an embryonic microcrack. As it follows from equation (10), always $L_m > L_c$ ($\zeta_m > \zeta_c$), i.e., the type II instability at the pile-up head occurs before the condition for the type I instability can be satisfied. Thus, it is the joining of two leading dislocations at the pile-up head that determines the criterion for the dislocational crack nucleation.

The explicit form of this criterion is rather complicated. But for the region of possible occurrence of type II instability, when type I instability is wittingly inaccessible, in accordance with equation (8) it will be $A < 1/(1 + S_2/S_2) < 1/2$. Then the components of force F_{B_2} at $\zeta = \zeta_m$ may be presented in the form of a power series expansion with respect to the small parameter A. Retaining in the expansion the terms not higher than the linear ones, we obtain the criterion of the microcrack nucleation at the head of the blocked dislocations pile-up **(6)**

$$n(\tau_t - \tau_i) = 0.308(g^*_m - \sigma_n) \quad (g^*_m = \tfrac{3}{4}g_m + \tfrac{1}{4}g_0 = \nu g_m, \quad \nu \leqslant 1) \tag{12}$$

Note that this criterion associates the fracture nucleation with cohesion in a specific cleavage plane which may be a grain boundary weakened by impurities. The obtained condition proves to be noticeably less severe than the initial Stroh criterion and its further refinements **(2)(4)**.

Dislocational crack growth

This stage of the pile-up evolution differs from the above by the fact that its leading element now will be a wedge-like dislocational crack – superdislocation $B_1 \geqslant 2b$ with non-interacting faces. Here we shall follow the conventional method of describing the cracks with small tip zones **(3)** and introduce an integral characteristic – the work of cleavage fracture $\gamma = \frac{1}{2}\int_0^\infty g(u)\,du$. Then $g_1(u_1)$ in the model equations is omitted and the dislocational crack shape is imposed by the condition known in the theory of cracks **(3)**, in our case this condition will take the form

$$\lim_{y \to -h_1} \sqrt{(y + h_1)}\eta_1(y) = \frac{2}{\pi}\sqrt{\left(\frac{\gamma}{M}\right)} \tag{13}$$

This mathematically differentiates the problem of the crack growth at the pile-up head from the previous one.

Interaction of the embryon crack B_1 with the remainder part of the pile-up was studied **(6)** in the approximation of the long-range stress field, i.e., assuming $\eta_2(y) = b\,\delta(y)$ (further for element B_1 index '1' in designations of its characteristics is omitted). Such formulation of the problem of interaction between the microcrack and pile-up is close to that described in **(2)**, but it is a more general one.

Equations (6) and (13) lead to the equation for the size of the dislocational crack

$$3(S_2 + S_3)h^2 + 4\sigma_n h - 16\sqrt{(M\gamma)}h^{1/2} + 8B_1 M = 0 \tag{14}$$

Its accurate solution is difficult. But from the analysis of the conditions for existence of its real roots it is possible to find the limit size h_c of a stable microcrack in the stress field

$$h_c = \frac{4M\gamma}{\sigma_n^2}\left\{1 - \sqrt{\left(1 - \frac{B_1\sigma_n}{\gamma}\right)}\right\}^2 \quad \left(\frac{B_1\sigma_n}{\gamma} \leqslant 1\right) \tag{15}$$

This gives a more definite solution to the condition of type I instability, equation (4). The analysis **(6)** showed that for the range of the possible type II instability at the head of the pile-up resting upon the crack we may approximately accept

$$h = \frac{1 - \sqrt{\{1 - 3h_c^2(S_2 + S_3)/(8B_1 M)\}}}{3h_c(S_2 + S_3)/(8B_1 M)} \tag{16}$$

Further the microcrack and pile-up interaction are considered similarly to that described above.

In accordance with equations (2), (6), (16) we find approximately **(6)**

$$F_{B_1B_2} = \frac{MbB_1}{L}\left[1 - \frac{g}{16}\kappa\frac{\chi(\zeta)}{\zeta^2}\right] + 0(\zeta^{-5}) \tag{17}$$

where, the same as before, $\zeta = L/h_c > 1$, $\chi(\zeta) = \{h(\zeta)/h_c\}^2$ and $\kappa = 4\gamma\{1 - \sqrt{(1 - B_1\sigma_n/\gamma)}\}/(B_1\sigma_n)$. Thus, we have a result similar to the previous section. Repeating the calculations described above and ignoring the terms with higher powers of the small parameter $b\sigma_n/\gamma < 1$ (this non-equality is broken down with such a large σ_n, that the dislocational crack with $B_1 = 2b$ will be unstable even in the absence of a pile-up), the condition of the next dislocation to drop into the embryon crack at $B_1 = 2b$ is found approximately in the form **(6)**

$$n(\tau_t - \tau_i) = 3.35(\gamma/b - 1.50\sigma_n) \tag{18}$$

The known results **(2)** allow to suppose that the critical stage of the dislocational crack growth is the pushing in of the next dislocation into the fracture embryon formed by joining of the first two ones. After this there comes the instability of the pile-up as a whole and its drop into the spreading microcrack, probably, up to the complete exhaustion of the pile-up. Then equation (18) presents the criterion for dislocational crack growth at the pile-up head.

Fracture of elasto–plastic solids: criterion and conditions of stress/strain controlled fracture

The microfracture model opens the way to build up the fracture criterion at a given material point in terms of the state macroparameters (stresses and strains) and some microstructural characteristics of the material, as well as for the analysis of the factors influencing the fracture mode and limit state of elasto-plastic solids.

Fracture criterion at a material point

We shall use the simplest method of building up the physical (structural) macromodels of the processes in solids. We consider that the active dislocations are localised in groups arranged in slip lines, the mean spacing of which is h_s. The initial number of dislocations in groups $n_0 = \omega\bar{\rho}_0 h_s$, where $\bar{\rho}_0$ is the initial density of dislocations in the material, factor ω is determined by the number of slip systems and the fraction of movable dislocations. Just at the stage of macro-elastic deformation, but when in any slip system $\tau_{xy} > \tau_i$, such groups can form blocked pile-ups. In the region of macroplastic straining the value of plastic shear strain in the system under consideration $\gamma_{xy}^{pl} = [u_x]/h_s$, where $[u_x] = n'b$ is the value of the plastic shear (displacement u_x discontinuity when passing over the line $y = 0$) produced by passing of n' dislocations. Then the capacities of the possible pile-ups – incomplete slips will reach the value $n = n_0 + [u_x]/b = n_0 + h_s\gamma_{xy}^{pl}/b$. The fracture event at a material point is assumed to be completed when for the most unfavourable system of glide-and-cleavage planes a more severe condition among those in equations (12) and (18) will be satisfied, i.e., when the complete breakdown of equilibrium stability of any fracture precursor at a material point will occur and the pile-up will turn into a dislocational crack. The fracture criterion at the elasto–plastic solid macropoint is presented in terms of the maximum values of plastic shear strain γ_{max}^{pl}, shear τ^{max} and normal σ_n^{max} stresses

$$(\varepsilon_{\rho 0} + \gamma_{max}^{pl})(\tau^{max} - \tau_i)/\hat{\gamma} = \hat{\sigma}(g_m, \sigma_n^{max})$$
$$(\varepsilon_{\rho 0} = \omega\bar{\rho}_0 b; \quad \hat{\gamma} = b/h_s; \quad \hat{\sigma} = \max\{0.308(g_m^* - \sigma_n^{max}); 3.35(\gamma/b - 1.5\sigma_n^{max})\}) \tag{19}$$

Here h_s or 'quantum' of plastic shear strain $\hat{\gamma}$ (when b is the 'quantum' of shear) reflects the dislocational inhomogeneity (micro-localisation) of plasticity. The form of equation (19) will be a little changed if the criterion is rewritten in terms of the macroscopic equivalent plastic strain ε_{eq}^{pl} and principal stresses $\sigma_1 > \sigma_2 > \sigma_3$.

Analysis of fracture behaviour

Depending on the value of the material microstructural characteristics $\varepsilon_{\rho 0}$ and $\hat{\gamma}$ the generally known phenomenological criteria of the maximum stress or critical strain may be obtained as the extreme cases of equation (19). Thus, e.g., equation (19) is reduced to the stress-type criterion at small $\hat{\gamma}$ and non-small (moderate) $\varepsilon_{\rho 0}$, such that $\varepsilon_{\rho 0}/\hat{\gamma} \gg 1$ and $\varepsilon_{eq}^{pl}/\varepsilon_{\rho 0} \ll 1$. The latter does not mean that the plastic deformation at rupture is obligatorily vanishingly small here, but as a particular case it is possible to fulfil the criterion at $\varepsilon_{eq}^{pl} = 0$. At smaller $\varepsilon_{\rho 0}/\hat{\gamma}$ the failure will need the increased (or large) plastic strain and the criterion will become a strain-type one.

The above refers to the invariable triaxiality of the stress state. Since equation (19) comprises both normal and shear stresses, the critical combination of the point mechanical state parameters ε_{eq}^{pl}, τ^{max}, σ_n^{max} will also depend upon the stress state shape: the higher is the stress triaxiality, the lower is the fracture strain, i.e. a more brittle fracture will be observed macroscopically (Fig. 3). But this is only one aspect of the ductile/brittle behaviour – macro-manifestation

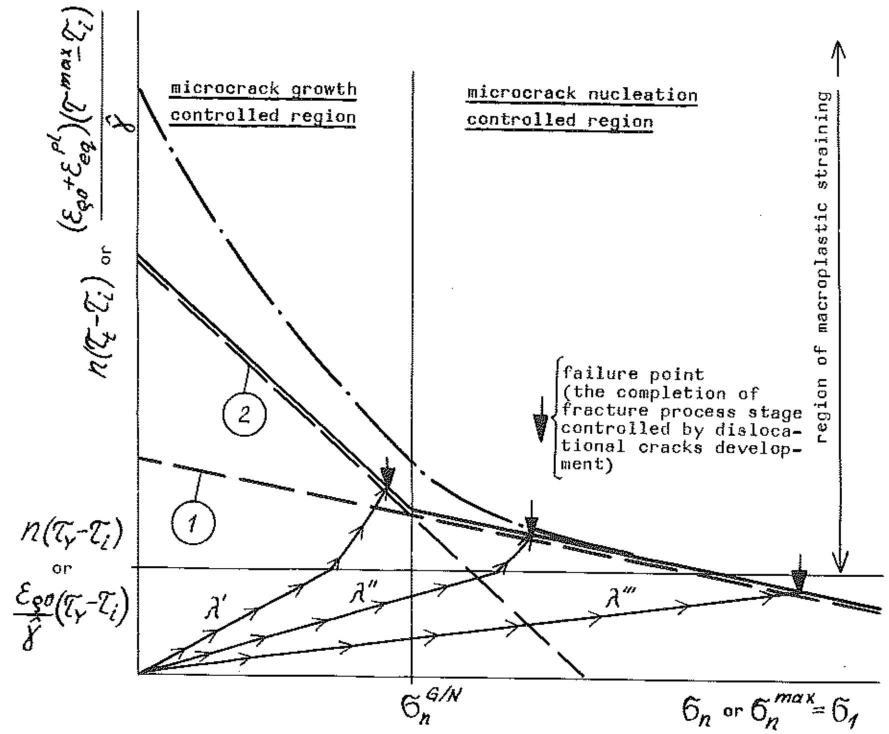

Fig 3 Fracture criteria in terms of micro- and macrovariables (parameters of pile-up and characteristics of stress–strain state and microstructure): broken lines – criteria of nucleation (1) and growth (2) of dislocational cracks, equation (12) and equation (18); solid line – criterion of instability of pile-up as a whole and of cleavage fracture completion at a material point, governed by dislocational cracks development, equation (19). Lines with arrows show the loading paths at the material point depending on the parameter of stresses triaxiality $\lambda = \sigma_3/\sigma_1$, whose values are $\lambda' < \lambda'' < \lambda$; horizontal line separates the region of the macroscopically elastic stage from the elasto–plastic one which comes when the macroscopic yield stress τ_Y is exceeded. In the space of material point state macroparameters the upper dash–dot line corresponds to full completion of rupture when the process is not limited to the stage of dislocational microcrack growth but is transferred into the region governed by the growth of microvoids.

which is not associated with variation of the fracture micromechanism by quasi-cleavage.

The second aspect will be found when the interrelation between the dislocational crack nucleation and growth is considered. Using the approximate relations – Orovan's formula $g_m^2 = E\gamma/b$ and the estimation for the BCC iron $g_m = 0.18E$ (see Ref. **(8)**) – we shall obtain the microfracture criteria curves corresponding to equation (12) and equation (18) as it is shown in Fig. 3. Respective to their mutual arrangement in the plane of the governing parameters the regions of fracture governed by growth or nucleation of microcracks are separated, the boundary between them being is determined by stress $\sigma_n^{G/N}$. For steels $\sigma_n^{G/N} \approx 2600$ MPa. In smooth tensile specimens even for high-strength steels the stresses do not obviously reach 2000 MPa. Here the fracture nuclei growth does not follow spontaneously their formation, i.e., the pile-ups equilibrium stability is kept and the fracture completion requires continuation of the plastic straining. In this case the dislocations density is increased as well as the probability of the opposite pile-up presence on the microcrack path. The latter leads to the premature transformation of the microcrack into a microvoid. The stage of the dislocational cracks (of quasi-cleavage type) development does not lead to completion of the rupture which is transferred to another microstructural level of ductile fracture by microvoid coalescence. Then the rupture completion requires the additional plastic strain for realisation of the further process stages. It will be another way, e.g., in fracture of solids with stress concentrators – notches or macrocracks – where tensile stresses even in steels of medium strength may exceed the value $\sigma_n^{G/N}$. Here more severe is the condition of microcracks nucleation, which, having just emerged, will spontaneously spread absorbing the pile-ups which have produced them. This will take place against the background of still relatively low dislocations density and, hence, at a lower probability of the crack blunting due to its intersection with a group of opposite-sign dislocations. Then the embryo crack propagation by cleavage will be wider, i.e. the fraction of quasi-cleavage will be higher and the fracture will be more brittle.

We hope the present paper has shown a more complete understanding of the prerequisites for ductile/brittle transitions will be achieved as a result of the analysis of elementary physical mechanisms, and this will help the development of quantitative metal science approaches to the creation of more efficient fracture-resistant microstructures.

Conclusions

An improved theoretical model of dislocational crack nucleation and growth in solids has been developed. Two leading elements of the Stroh-type blocked array of edge dislocations were considered individually and the effects of their cores were taken into account. These cores were treated as wedge-like discontinuities with their faces mutually attracted according to the solid cohesive forces law. The equilibrium stability of such a dislocational configuration under the action of shear stress τ_{xy} in the array glide plane and of tensile stress σ_{xx} in the plane of expected cleavage was analysed. This approach opened the way for a unified treatment of both stages of the microfracture process – nucleation and growth of dislocational cracks.

Two alternative conditions of the equilibrium stability loss at the pile-up head were analysed: (i) the Griffith type instability of the array head element (i.e., cleavage of the single lattice dislocation or superdislocation-embryonic wedge-like crack if it had nucleated) due to tensile stress, and (ii) the positional instability of neighbouring lattice dislocation resulting in its joining with the head (super) dislocation. As a result, the nucleation and growth of the microcrack was shown to occur by successive joining of the array dislocations at its head due to attractive short-range core-caused component of the dislocations' interaction force. Quantitative criteria of microcrack nucleation and growth were derived in which the role of local cohesive forces in fracture cores and of both external stresses (shear and tensile) are reflected.

Using the approach of combined micro- and macro-mechanics, the respective macroscopic fracture criterion in a material point was obtained in terms of continuum variables of maximum shear and tensile stresses $\tau^{max} = (\sigma_1 - \sigma_3)/2$ and $\sigma_n^{max} = \sigma_1$, and equivalent plastic strain ε_{eq}^{pl}, where some mechano-structural characteristics of solids were included. Depending on the specific values of the latter, the usual phenomenological failure criteria of maximum stress or critical strain were shown to be the limit cases of the proposed criterion.

The results of the investigation undertaken were applied to the analysis of factors governing the transition from stress- to strain-controlled fracture and from more to less ductile (brittle) behaviour of the given material depending on its intrinsic properties (cohesion in fracture cores and dislocational processes heterogeneity) and stress–strain state (stresses triaxiality) in the solid.

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