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Theoretical analysis of ductile-brittle transition

R. B. PĘCHERSKI (WARSZAWA)

THE AIM of the paper is to propose a local ductile-brittle transition criterion with an account of scale effect and stress multiaxiality. It is based on the analysis of microscopic mechanisms of brittle fracture and a detailed analysis of the statistical effect and stress state factor as well. Also a method of calculation of ductile-brittle transition temperature is discussed.

Celem pracy jest sformułowanie lokalnego kryterium kruchego przejścia z uwzględnieniem efektu skali i złożoności stanu naprężenia. Wykorzystano przy tym analizę mikroskopowych mechanizmów kruchego pękania i szczegółową analizę efektu statystycznego oraz współczynnika stanu naprężenia. Zaproponowano również metodę określenia temperatury kruchego przejścia.

Целью работы является формулировка локального критерия хрупкого перехода с учетом эффекта масштаба и сложности напряженного состояния. При этом использован анализ микроскопических механизмов хрупкого растрескивания и подробный анализ статистического эффекта, а также коэффициента напряженного состояния. Предложен тоже метод определения температуры хрупкого перехода.

1. Introduction

THE PLASTIC properties of bcc metals are very sensitive to strain rate and temperature. This is manifested in an increase in yield strength and decrease in ductility when temperature decreases or strain rate increases. It is then required that the range of the exploitation temperature of many engineering components be limited by the Nil Ductility Transition Temperature. This temperature is usually determined in standard tests for standardized specimens. The method provides satisfying results for comparing different materials but does not supply adequate information on the ductile-brittle transition temperature characteristic of a whole body. The Nil Ductility Temperature for an engineering component is usually estimated empirically on the basis of the standard test results and a range of correction factors. Such a method is rather ambiguous and bears many limitations. In the author's opinion these shortcomings might be cleared up by means of a theoretical analysis of the ductile-brittle transition.

The paper is devoted to the formulation of a local criterion of ductile-brittle transition and a method of derivation of transition temperature with an account of scale effect and stress multiaxiality. The criterion is based on the analysis of microscopic mechanisms of brittle fracture and statistical effect as well. Scale effect is taken into account with a view of the concept of a certain characteristic volume, while stress multiaxiality is defined by a stress state factor. The derivation of transition temperature for a whole body requires the solution of a suitable mechanical problem with temperature effects.

2. Physical motivations

The microscopic mechanisms of brittle fracture have been investigated by such authors as COTTRELL [1], KNOTT [9], PETCH [16], TETELMAN, MC EVILY [22], and YOKOBORI [28]. The author's paper (PĘCHERSKI [17]) was also devoted to the detailed analysis of the experimental and physical foundations of ductile-brittle transition as well as related mechanisms of plastic deformation in mild steel. On the basis of the results mentioned above the following general conclusions can be drawn.

The initial stage of brittle fracture is the nucleaction of microcracks in single grains. It is preceded by a local, nonhomogeneous, plastic deformation realized in separate grains by slip or twinning. The mechanisms of cleavage is governed, therefore, by motion and pile-up of dislocations on sufficiently strong obstacles. As a result of this, a severe local stress concentration arises. In certain circumstances (low temperature, high strain rate, neutron irradiation) cleavage may occur in neighbouring grains.

The second stage of brittle fracture is the growth and noncontinuous propagation of microcracks. Finally, they join in a macrocrack which may be responsible for failure of a structural member. The propagation of microcracks occurs in cleavage planes similar to a surface perpendicular to the lines of the maximum tension stress. Thus the critical point of brittle fracture is the propagation of a microcrack preceded by local plastic deformation.

Consequently, it is evident that the necessary condition of brittle fracture is an unstable growth of microcrack. The suitable criterion was formulated by COTTRELL [1] and, independently, by PETCH [16]:

$$(\sigma_i d^{1/2}+K_y)K_y \geqslant \beta\mu\gamma_e, \tag{2.1}$$

where μ denotes the elastic shear modulus, γ_e is the density of the effective surface energy, σ_i, K_y are the "friction" stress responsible for dislocation motion in suitable glide planes within a singular grain and the grain size factor in the Hall-Petch relation, respectively. The coefficient β determines three states of stress for which the criterion (2.1) is valid:

$$\beta = \begin{cases} 1, & \text{for tension,} \\ 2, & \text{for torsion,} \\ 1/3, & \text{for notched bar.} \end{cases} \tag{2.2}$$

The criterion (2.1) is very useful for qualitative analysis of the ductile-brittle transition process but has some disadvantages from the practical point of view. First of all, the criterion is valid only for single crystals or pure polycrystals (cf. TETELMAN, MC EVILY [22]). It is formulated in microscopic quantities which are difficult to determine experimentally. Furthermore, it is applicable only for small specimens in three special states of stress.

3. Formulation of ductile-brittle transition criterion

The remarks mentioned above substantiate the necessity of further search for a new ductile-brittle transition criterion which would be valid for technical alloys, e.g. carbon steel, and would be applicable in the analysis of the real structural member in a complex state of stress.

The susceptibility to brittle fracture is strongly dependent on the state of stress, the stress concentration and nonhomogeneity as well as the size of the body. The scale effect is manifested in a statistical effect and in an amount of the stored elastic energy which is released during the fracture process. In the case of the local growth of a microcrack, the statistical effect is of great importance. The stored elastic energy plays a substantial role during macrocrack propagation and failure of a whole structure. The statistical effect may be shortly explained in the following way.

Nonhomogeneity is characteristic of all real materials. The larger the body, the greater the probability that there exists such a site in which suitable local stress concentration, nucleation and critical growth of microcrack occur. Thus, for the same concentration of nonhomogeneity the probability of fracture increases with increasing volume (cf. FREUNDENTHAL [2]).

In conclusion, it is assumed that the most important factors affecting the local growth of microcrack are:

(i) the maximum principal tension stress $\sigma_1 > 0$;

(ii) the stress state factor which in the case of the body without macroscopic stress concentrators is equal to

$$\Pi = \frac{\sigma_{eq}}{\sigma_1}, \tag{3.1}$$

where

$$\sigma_{eq} = f(\sigma_1, \sigma_2, \sigma_3) \tag{3.2}$$

is the equivalent stress which is a certain scalar function of the principal stresses;

(iii) the plastic stress concentration factor in the case of the body with macroscopic stress concentrators

$$K_{\sigma(p)} = \frac{\sigma_1^p}{\sigma_Y}, \tag{3.3}$$

where σ_1^p, σ_Y are the maximum tension stress in a local plastic zone and tensile yield strength, respectively;

(iv) the volume of the most severely stressed part of the body V_k. This is the characteristic volume necessary for suitable local stress concentration and growth of microcrack.

In our further consideration two cases will be dealt with. First, a criterion of ductile-brittle transition for a body without macroscopic stress concentrators is proposed. Then a suitable criterion for a notched body is formulated.

In the first case, the ductile-brittle transition occurs if in the volume V_k the yield limit is reached:

$$\sigma_{eq} = \sigma_Y \tag{3.4}$$

and the inequality

$$\sigma_1 \geqslant \sigma_F(V_k) \tag{3.5}$$

in the volume V_k is satisfied. The symbol $\sigma_F(V_k)$ denotes the fracture strength corresponding to the critical volume V_k.

The criterion takes a more compact form when the definition of the stress state factor Π, given by Eq. (3.1), is used:

$$\sigma_Y \geqslant \sigma_F(V_k)\Pi \quad \text{in} \quad V_k. \tag{3.6}$$

This inequality means that the ductile-brittle transition occurs provided the tensile yield strength attains in the volume V_k the value of the critical fracture strength determined by the material properties, the volume V_k, and the state of stress.

As an example of the specification of the function $\sigma_F(V_k)$ we may assume that the size effect is described by the classical Weibull relation

$$\sigma_F = \sigma_f^*\left(\frac{V^*}{V_k}\right)^{\frac{1}{n}}, \quad V_k > V^*, \quad n > 1, \tag{3.7}$$

where σ_f^* is the local macroscopic cleavage strength pertaining to the elementary volume V^* and n denotes the Weibull nonhomogeneity coefficient.

The local cleavage strength σ_f^* is a measure of material resistance against microcrack growth. The concept of σ_f^* was introduced by OROWAN [14], HENDRICKSON *et al.* [5] and KNOTT, COTTRELL [8]. These authors investigated the fracture modes of a notched specimen in low temperatures and found that brittle fracture always occurs after the tension stress exceeds a certain critical value locally in a small zone beneath the notch root. This idea was further developed by KNOTT [6, 7], WULLAERT [27], GRIFFITHS, OATES [3], OATES [12, 13], TETELMAN *et al.* [23], [24], RAU, TETELMAN [19], GRIFFITHS, OWEN [4], RICHTIE *et al.* [20] and PARKS [15]. It was proved experimentally that the local cleavage strength σ_f^* is relatively independent of the strain rate and the temperature.

The quantity σ_f^* can be determined on the basis of the results of an instrumented Charpy test, and an analysis of stress distribution in the local plastic zone beneath the notch root. In the papers of MALKIN, TETELMAN [11], WILSHAW *et al.* [26] the relation between σ_f^* and the critical fracture toughness K_{Ic} was established:

$$K_{Ic} = 2.96\sigma_Y\left[\exp\left(\frac{\sigma_f^*}{\sigma_Y}-1\right)-1\right]^{1/2}\sqrt{\varrho} \tag{3.8}$$

provided that $\varrho \geqslant \varrho_0$, where ϱ_0 is the minimum value of the notch root radius dependent on the material microstructure. Thus, for given values of K_{Ic}, σ_Y and ϱ_0 the local cleavage strength σ_f^* may be determined:

$$\sigma_f^* = \sigma_{LY}\left\{1+\ln\left[1+\frac{\varrho_0}{2.96}\left(\frac{K_{Ic}}{\sigma_Y}\right)^2\right]\right\}. \tag{3.9}$$

It is worth mentioning that the quantities σ_f^*, V^* are determined by the microstructure only, primarily by the grain size and the distribution of second phase particles. Thus they are the material parameters independent of specimen geometry. The question arises as how to evaluate the quantity V^*.

The volume V^* should contain such a number of grains which is sufficient for microcrack growth. It is possible to estimate the quantity V^* basing on theoretical models of microcrack growth as well as on microscopic observations.

A simplified method of the calculation of an elementary volume was proposed by TETELMAN *et al.* [24]

$$V_s^* = \begin{cases} 4d\varrho t, & \varrho \geqslant 2d, \\ 8d^2 t, & \varrho < 2d, \end{cases} \tag{3.10}$$

where t denotes the specimen thickness and ϱ is the radius of the notch root. As a matter of fact, V_s^* defined by Eq. (3.10) depends on the notch root radius and the specimen thickness. To be precise we should connect with V_s^* the cleavage strength $\sigma_{f_s}^*$ determined by the following relation:

$$\sigma_{f_s}^* = \sigma_f^* \left(\frac{V^*}{V_s^*} \right)^{\frac{1}{n}}. \tag{3.11}$$

From Eqs. (3.7) and (3.11) the following relation for the fracture strength σ_F corresponding to the characteristic volume V_k is obtained:

$$\sigma_F = \sigma_{f_s}^* \left(\frac{V_s^*}{V_k} \right)^{\frac{1}{n}}. \tag{3.12}$$

Let us remark that σ_F is referred now to the quantities $\sigma_{f_s}^*$, V_s^*, which depend on size and specimen geometry. However, for suitably small specimens we may assume that

$$\left(\frac{V^*}{V_s^*} \right)^{\frac{1}{n}} \approx 1 \quad \text{and} \quad \sigma_{f_s}^* \approx \sigma_f^*. \tag{3.13}$$

The maximum admissible value of the specimen thickness t should be determined experimentally.

In the case of a body with macroscopic concentrators the ductile-brittle transition criterion takes the form

$$\sigma_Y \geqslant \sigma_F(V_k) \frac{1}{K_{\sigma(p)}}, \tag{3.14}$$

which follows from Eqs. (3.3) and (3.5). The volume V_k now corresponds to the region beneath the notch root in which the maximum tension stress σ_1 is higher than the cleavage strength σ_f^*.

The crucial point in the determination of the characteristic volume V_k in both cases is the demand that the distance along which the stress σ_1 is higher than σ_f^* be equal to the double grain diameter or a mean space between second phase particles. On the other hand the range of applicability of the macroscopic theory of plasticity should be taken into account (cf. PĘCHERSKI [18]).

Taking into consideration Eqs. (3.6), (3.7) and (3.14) the general criterion for both cases becomes

$$\sigma_Y \geqslant \sigma_f^* \left(\frac{V^*}{V_k} \right)^{\frac{1}{n}} \Sigma, \quad V_k > V^*, \quad n > 1, \tag{3.15}$$

where

$$\Sigma = \begin{cases} \Pi & \text{for the body without macroscopic concentrators,} \\ \dfrac{1}{K_{\sigma(p)}} & \text{for the body with macroscopic concentrators.} \end{cases} \tag{3.16}$$

Thus ductile-brittle transition depends on the macroscopic quantities σ_Y, σ_f^*, V^*, n, depending on material only, the characteristic volume V_k and the state of stress, as well.

The Weibull nonhomogeneity coefficient n may be determined experimentally using normalized specimens with different thickness t_1, t_2. In such a case we have:

$$V_1^* = \begin{cases} 4d\varrho t_1, & \varrho \geqslant 2d, \\ 8d^2 t_1, & \varrho < 2d, \end{cases} \qquad V_2^* = \begin{cases} 4d\varrho t_2, & \varrho \geqslant 2d \\ 8d^2 t_2, & \varrho < 2d. \end{cases} \tag{3.17}$$

Due to the fact that

$$\sigma_{f_1}^* = \sigma_{f_2}^* \left(\frac{V_2^*}{V_1^*} \right)^{\frac{1}{n}} = \sigma_{f_2}^* \left(\frac{t_2}{t_1} \right)^{\frac{1}{n}}, \tag{3.18}$$

we have

$$n = \frac{\log \dfrac{t_2}{t_1}}{\log \dfrac{\sigma_{f_1}^*}{\sigma_{f_2}^*}}. \tag{3.19}$$

Let us consider the examples of the specification of the stress state factor Π.

In the simplest nontrivial case we may assume that the equivalent stress σ_{eq} is given according to the Tresca yield condition by the following relation:

$$\sigma_{eq}^T = \sigma_1 - \sigma_3. \tag{3.20}$$

In such a case the stress state factor is equal to

$$\Pi_T = \frac{\sigma_{eq}^T}{\sigma_1} = 1 - \varkappa_2, \tag{3.21}$$

where

$$\varkappa_2 = \frac{\sigma_3}{\sigma_1}. \tag{3.22}$$

Assuming that according to the Huber-Mises yield condition σ_{eq} is given by

$$\sigma_{eq}^H = \sigma_i = \frac{1}{\sqrt{2}} [(\sigma_1 - \sigma_2)^2 + (\sigma_1 - \sigma_3)^2 + (\sigma_2 - \sigma_3)^2]^{1/2}, \tag{3.23}$$

where σ_i denotes the stress intensity, the Schnadt stress state factor will be obtained (cf. SCHNADT [21]):

$$\Pi_H = \frac{\sigma_i}{\sigma_1} = (1 + \varkappa_1^2 + \varkappa_2^2 - \varkappa_1 - \varkappa_2 - \varkappa_1 \varkappa_2)^{1/2}, \tag{3.24}$$

where

$$\varkappa_1 = \frac{\sigma_2}{\sigma_1}. \tag{3.25}$$

In the third case the equivalent stress σ_{eq} proposed by LEBEDYEV and NOVIKOV [10] is used. The latter found experimentally that at normal temperatures yield of carbon steel is satisfactorily described by the Huber-Mises condition. At lower temperatures, however, they observed a change in the shape of the limiting surface. Namely, the relative resistance to strain decreases in the range of biaxial tension and increases in the range of tension-compression. The test results show that the widening of the limiting surface at lower temperatures develops nonisotropically and a systematic variation of the surface shape takes place in addition to widening. On the basis of probabilistic considerations, Lebedyev and Novikov formulated the following relation for the equivalent stress:

$$\sigma^L_{eq} = \chi\sigma_i + (1-\chi)\sigma_1 A^{1-I}, \tag{3.26}$$

where $\chi = \dfrac{\sigma_t}{\sigma_c}$, $A = 1-\dfrac{1}{n}$ are constants depending on material properties at a given temperature, n is the Weibull nonhomogeneity coefficient, σ_t, σ_c are the tension and compression yield strength, and $I = \dfrac{\sigma_1+\sigma_2+\sigma_3}{\sigma_i}$ is the parameter of loading severity.

In such a case the stress state factor is given by the following relation:

$$\Pi_L = \frac{\sigma^L_{eq}}{\sigma_1} = \chi\Pi_H + (1-\chi)A^{\frac{1+\varkappa_1+\varkappa_2}{\Pi_H}} \tag{3.27}$$

Let us remark that for $\chi = 1$ the former relation for the stress state factor is obtained.

4. Derivation of the ductile-brittle transition temperature

The inequality (3.15) is useful in an analysis of the influence of different parameters (e.g. the temperature ϑ, the second invariant of the strain rate tensor I^{ξ}_2) on the ductile-brittle transition process. The parameters σ^*_f, V^*, n are assumed to be dependent on the material structure only, whereas the quantities k_Y, V_k, Σ are the functions of ϑ and I^{ξ}_2. In order to determine the characteristic volume V_k and the stress state factor Σ, a suitable mechanical problem with temperature effects must be solved. The quantity V_k is calculated after determining the first yielding site. The requirements of the minimum plastic zone size, discussed before, must be taken into account by that. Then, for the loading process which induces the plastic zone containing the volume V_k, the stresses and the coefficient Σ are calculated(1). The loading process is the fictitious one which allows to test the behaviour of the body in extreme conditions. The ductile-brittle transition temperature appears to be a suitable parameter characterizing the behaviour of the body. In such a case the criterion (3.15) takes the form

$$\sigma_Y(\vartheta_k, I^{\xi}_2) = \sigma^*_f\left[\frac{V^*}{V_k(\vartheta_k, I^{\xi}_2)}\right]^{\frac{1}{n}}\Sigma(\vartheta_k, I^{\xi}_2). \tag{4.1}$$

(1) An example of similar calculations and derivation of ductile-brittle transition temperature for a spherical vessel under neutron irradiation is given in the author's paper (PĘCHERSKI [18]).

This is the equation for the transition temperature ϑ_k. In many practical cases the fracture strength

$$\sigma_f = \sigma_f^* \left(\frac{V^*}{V_k}\right)^{\frac{1}{n}} \Sigma \tag{4.2}$$

may be assumed as independent of the temperature. Thus the following equation for ϑ_k should be solved:

$$\sigma_Y(\vartheta_k, I_2^p) = \sigma_f^* \left[\frac{V^*}{V_k(I_2^p)}\right]^{\frac{1}{n}} \Sigma(I_2^p). \tag{4.3}$$

In most practical cases Eq. (4.3) gives satisfactory results.

In the analysis of the ductile-brittle transition it is reasonable to neglect strain hardening and assume the model of an elastic-ideally viscoplastic material. In such a case the dynamic yield condition takes the form (cf. PĘCHERSKI [17]),

$$\sqrt{J_2} = k_0(\vartheta) + A_1(\vartheta)\Phi^{-1}\left(\frac{\sqrt{I_2^p}}{\eta_1}\right) \tag{4.4}$$

for the case of the Huber-Mises yield condition, the thermally activated plastic flow corresponding to the shear strain rates $\dot{\gamma}^p = 2\sqrt{I_2^p} \in (10^{-5} \div 5\times 10^3)\mathrm{s}^{-1}$, and low temperatures. The symbol J_2 denotes the second invariant of the stress tensor. The dynamic yield strength consists of the temperature-dependent quasi-static shear strength $k_0(\vartheta)$ and the part sensitive to the strain rate where $A_1(\vartheta)$ is the temperature-dependent material function, Φ is the excess stress function and η_1 is the viscosity coefficient. Similarly, in the case of viscous drag mechanisms corresponding to higher strain rates $\dot{\gamma}^p > 5\times 10^3\ \mathrm{s}^{-1}$, the dynamic yield condition takes the form (cf. PĘCHERSKI [17])

$$\sqrt{J_2} = k_0(\vartheta) + A_1(\vartheta)\Phi^{-1}\left(\frac{\frac{1}{2}\dot{\gamma}_0^p}{\eta_1}\right) + \frac{\sqrt{I_2^p} - \frac{1}{2}\dot{\gamma}_0^p}{\eta_2}. \tag{4.5}$$

In this case the dynamic shear yield strength depends linearly on the second invariant of the strain rate.

In many practical cases the following specification of the material functions

$$\begin{aligned} k(\vartheta) &= k_0 - \alpha_2\vartheta\log\eta_1, \quad A_1(\vartheta) = -\alpha_2\vartheta, \\ \Phi(\cdot) &= \exp(\cdot) \end{aligned} \tag{4.6}$$

is justified physically and experimentally as well.

The criterion of ductile-brittle transition takes now the following form:

$$k_0 + \alpha_2\vartheta_k\log\sqrt{I_2^p} - \alpha_2\vartheta_k\log\eta_1 = \frac{1}{\sqrt{3}}\sigma_f, \tag{4.7}$$

$$k_0 + \alpha_2\vartheta_k\log\sqrt{\frac{1}{2}\dot{\gamma}_0^p} - \alpha_2\vartheta_k\log\eta_1 + \frac{\sqrt{I_2^p} - \frac{1}{2}\dot{\gamma}_0^p}{\eta_3} = \frac{1}{\sqrt{3}}\sigma_f \tag{4.8}$$

for the strain rates $\dot{\gamma}^p \in (10^{-5}-5\times10^3)\ \mathrm{s}^{-1}$ and $\dot{\gamma}^p > 5\times10^3\ \mathrm{s}^{-1}$, respectively. From Eqs. (2.17) and (4.8) the relations for the ductile-brittle transition temperature ϑ_k may be obtained

$$\frac{1}{\vartheta_k} = \frac{\alpha_2 \log \eta_1}{k_0 - \sigma_f} - \frac{\alpha_2}{k_0 - \frac{1}{\sqrt{3}}\sigma_f} \log \sqrt{I_2^p}, \tag{4.9}$$

$$\vartheta_k = \frac{1}{\alpha_2 \log\left(\frac{2\eta_1}{\dot{\gamma}_0^p}\right)} \left[k_0 - \frac{1}{\sqrt{3}}\sigma_f + \frac{1}{\eta_3}\left(\sqrt{I_2^p} - \frac{1}{2}\dot{\gamma}_0^p\right)\right] \tag{4.10}$$

for

$$k_0 > \sigma_f, \quad \eta_1 > \frac{1}{2}\dot{\gamma}_0^p.$$

In Eq. (4.9) the inverse of the transition temperature $1/\vartheta_k$ depends linearly on $\log \sqrt{I_2^p}$ whereas in Eq. (4.10) the transition temperature ϑ_k depends linearly on $\sqrt{I_2^p}$. The first dependence has been confirmed experimentally (cf. VITMAN, STEPANOV [25]) while the region of higher strain rates has not, according to the author's knowledge, been explored experimentally.

The relations (4.9) and (4.10) also determine the dependence of the transition temperature ϑ_k on the characteristic volume V_k, the stress state factor Σ and the critical cleavage strength σ_f^* as well. From Eqs. (4.9) and (4.10) we have:

$$\vartheta_k(V_k) = \vartheta_k(V^*) + \frac{\sigma_f^* \Sigma}{S}\left[1 - \left(\frac{V^*}{V_k}\right)^{\frac{1}{n}}\right], \tag{4.11}$$

where

$$S = \begin{cases} \alpha_2 \log \dfrac{\eta_1}{\sqrt{I_2^p}}, & \dot{\gamma}^p < \dot{\gamma}_0^p, \\ \alpha_2 \log \dfrac{2\eta_1}{\sqrt{\dot{\gamma}_0^p}}, & \dot{\gamma}^p \geqslant \dot{\gamma}_0^p. \end{cases} \tag{4.12}$$

5. Concluding remarks

The applicability of the proposed method of derivation of transition temperature requires more experimental investigations concerning the determination of the material parameters σ_f^*, n and V^*.

The discussed ductile-brittle transition temperature pertains to the ideal model of a structural member. The existence of internal stresses and stress concentration produced in a technological process have been neglected in the model. The ductile-brittle transition temperature of a real structural member is equal to

$$\vartheta_{DBTT} = \vartheta_k + \Delta\vartheta_k, \tag{5.1}$$

where $\Delta\vartheta_k$ is the transition temperature increase caused by technological factors. The value of $\Delta\vartheta_k$ should be determined experimentally.

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