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# THE KEY PROBLEMS OF LOCAL APPROACH TO CLEAVAGE FRACTURE

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Based on the suggested multi-scale model of Local Approach (LA) to fracture, four main problems of LA are considered, namely: (i) the effect of micro-stress fluctuations on the crack nuclei instability; (ii) intensity of micro-crack nucleation and its influence on fracture probability; (iii) theoretical and experimental assessment of the value of threshold stress; (iv) stochastic analysis of "multi-barrier" effect at micro-crack growth in polycrystalline metal.

*Key words:* local approach to fracture, multi-scale model, local fracture stress

## 1. Introduction

The Local Approach to fracture (LA) has been significantly developed for the last three decades. This approach has enabled not only to clarify the nature and micromechanism of metal fracture, but also to describe the effect of loading conditions on the fracture limit of structures, which cannot be easily realized with the conventional global approach (Pineau, 2006; Pineau and Benoot, 2010; Bordet *et al.*, 2005; Beremin 1983, Margolin *et al.*, 1998). However, recent findings have demonstrated limitation of the conventional version of LA both in the theoretical and applied sense. This is due, first of all, to unnecessarily oversimplified description of the fracture process in Beremin's version of LA and its further modifications. Simultaneously with this version, the multi-scale approach to brittle fracture was offered in Kotrechko (1995, 2002, 2003), Kotrechko and Meshkov (2001), Kotrechko *et al.* (2007). Specific feature of this approach lies in possibility to describe regularities of a pre-cracked solid on macroscopic scale based on realistic physical models of the crack nuclei (CN) creation and instability in polycrystalline metals and alloys. This version of LA is more sophisticated for practical use; however, it may be applied as the theoretical basis for further development of conventional LA. This paper is aimed at consideration of key problems of LA, namely:

- accounting for the effect of stochastic micro-stress field on the CN instability in polycrystalline aggregate;
- prediction of the effect of plastic strain and temperature on the CN generation;
- theoretical and experimental determination of the value of threshold stress;
- properties and experimental determination of the local fracture stress;
- analysis of "multiple-barrier" effect at the CN propagation in polycrystal.

## 2. Crack nuclei instability

The Griffith criterion is conventionally used for description of the beginning of macro-crack unstable growth. However, most works do not account that the CN becomes unstable under the influence of *micro-stresses*. Only macroscopic stresses are usually considered. Pineau and Bennot

(2010) noted that the effect of micro-stresses should be accounted because it is the reason for both scatter of fracture stress and the value of statistical scale effect. The statistical model of cleavage fracture of a polycrystalline metal, in which the CN instability in stochastic micro-stress field is considered, was suggested in Kotrechko (1995). Microstresses in polycrystalline aggregate are characterized by a wide spectrum of amplitudes and wave lengths. Therefore, at modelling, two components were accounted separately, namely: (1) the microstresses $\xi_{ij}$ produced by grain-to-grain elastic misfit and (2) the microstresses $\xi_{ij}^p$ due to dislocations. In the first approximation, the microstresses $\xi_{ij}$ may be considered as homogeneous within the grain and changing from a grain to grain. The statistical distribution of these stress values may be approximated with sufficient accuracy by the normal law. The values of variances of these microstresses $D_{\xi_{11}}$, $D_{\xi_{22}}$, $D_{\xi_{33}}$ are functions of principal macro-stresses $\sigma_1$, $\sigma_2$, $\sigma_3$, and the mean values $\xi_{11}$, $\xi_{22}$, $\xi_{33}$ are equal to $\sigma_1$, $\sigma_2$, $\sigma_3$, respectively

$$\begin{aligned} D_{\xi_{11}} &= D_I\sigma_1^2 + D_{II}(\sigma_2^2+\sigma_3^2) + 2[\mu_I(\sigma_1\sigma_2+\sigma_1\sigma_3) + \mu_{II}\sigma_2\sigma_3] \\ D_{\xi_{22}} &= D_I\sigma_2^2 + D_{II}(\sigma_1^2+\sigma_3^2) + 2[\mu_I(\sigma_2\sigma_1+\sigma_2\sigma_3) + \mu_{II}\sigma_1\sigma_3] \\ D_{\xi_{33}} &= D_I\sigma_3^2 + D_{II}(\sigma_2^2+\sigma_1^2) + 2[\mu_I(\sigma_3\sigma_1+\sigma_3\sigma_2) + \mu_{II}\sigma_1\sigma_2] \end{aligned} \tag{2.1}$$

where $D_I = 1.7\cdot 10^{-2}$, $D_{II} = \mu_{II} = 0.66\cdot 10^{-2}$, $\mu_I = 0.72\cdot 10^{-2}$ for polycrystalline iron and Fe-based alloys.

From (2.1) it follows that even at *uniaxial macroscopic* tension ($\sigma_1 > 0$, $\sigma_2 = \sigma_3 = 0$), the *microscopic* stress state is *triaxial* ($\xi_{11} > 0$, $\xi_{22} \neq 0$, $\xi_{33} \neq 0$). In this case, for iron, the value of microscopic stress $\xi_{11}$ changes from $0.6\sigma_1$ to $1.4\sigma_1$, and the values $\xi_{22}$ and $\xi_{33}$ change from $-1.24\sigma_1$ to $+1.24\sigma_1$. This specific feature is one of the reasons for scatter of cleavage fracture on macroscopic scale, but it does not account in most conventional models.

Micro-stress fields induced by dislocations are significantly inhomogeneous, so, the effect of such fields may be described by the effective stress $\overline{\xi}$ (Indenbom, 1961)

$$\overline{\xi} = \frac{2}{\pi a}\int\limits_0^a \xi_{11}^p(x)\sqrt{\frac{x}{a-x}}dx \tag{2.2}$$

where $a$ is the CN length, $\xi_{11}^p(x)$ is the distribution function for tensile micro-stress along the path of microcrack growth.

The essence of this dependence is that micro-stresses support a crack growth if they change according to the law $1/\sqrt{x}$ with distance $x$ change. In Kotrechko (1995), the expression for $\overline{\xi}$ induced by the layer of randomly distributed dislocations near the grain boundary where the CN forms was obtained. The values of these stresses increase with plastic strain $\overline{e}$ growth. However, the critical value $e_c$ exists, at exceeding of which $\overline{\xi}$ decreases. As it is exhibited in Kotrechko (2002), Kotrechko *et al.* (1995, 2007), for typical structural steels $e_c \approx 0.02$. At $\overline{e} < e_c$, the dependence of $\overline{\xi}$ on strain may be approximated as

$$\overline{\xi} = k_\xi\sqrt{\frac{\overline{e}}{d}} \tag{2.3}$$

where $k_\xi$ is the coefficient (for $\alpha$-Fe and carbon steels it is equal to $\approx 16.8\,\mathrm{MPa}\sqrt{\mathrm{m}}$); $\overline{e}$ is the equivalent macro-plastic strain; $d$ is the grain size.

At strain $e_c < e \leqslant 0.2$, the expression for $\overline{\xi}$ is the following[1]

$$\overline{\xi} = k_\xi\sqrt{\frac{\overline{e}}{d}} - k_e\Big(\frac{\overline{e}}{e_c} - 1\Big) \tag{2.4}$$

[1]For typical ferritic steels $e_c \approx 0.02$.

where $k_e$ is the coefficient (for $\alpha$-Fe and carbon steels it is approximately equal to $40\,\mathrm{MPa}\sqrt{\mathrm{m}}$).

As it is shown in Kotrechko *et al.* (1995, 2007), Kotrechko (2003), the effect of dislocation micro-stresses on the CN instability results in a non-monotonic dependence of critical fracture stress $\sigma_f$ on the value of plastic strain (Fig. 1).

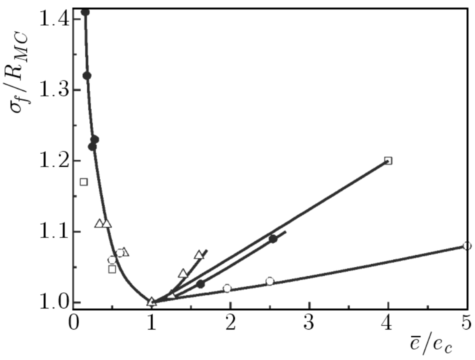


Fig. 1. Effect of plastic strain on the value of cleavage fracture stress $\sigma_f$ under uniaxial tension: $e_c$ is the critical value of plastic strain corresponding to the minimum level of brittle strength of metal $R_{MC}$ at uniaxial tension

With account of these regularities, the expression for critical stress of the CN instability on microscopic scale $\xi_c$ is the following

$$\xi_c = \Big(\frac{k_{Ic}}{\sqrt{a}} - \overline{\xi}\Big)\varphi(\theta,\eta) \tag{2.5}$$

where $k_{Ic}$ is the critical value of the stress intensity coefficient for the CN; $\varphi(\theta,\eta)$ is the function describing the effect of CN orientation and the micro-stress state mode on the value of $\xi_c$. In 2D-approximation

$$\varphi(\theta,\eta) = \frac{1}{\sqrt{\cos^2\alpha + \eta\sin^2\alpha}} \tag{2.6}$$

where $\alpha$ is the angle between the normal to crack plane and $\xi_{11}$ direction; $\eta$ is the parameter of the micro-stress state mode $(\eta = \xi_{22}/\xi_{11})$.

Equation (2.5) with account of (2.1) enables one to predict the value of *macroscopic* fracture stress $\sigma_f$ based on the criterion of CN instability on *microscopic* scale

$$\xi_{11} \geqslant \xi_c \tag{2.7}$$

As it is exhibited in Kotrechko (1995, 2002), Kotrechko *et al.* (2001), the probability of instability of one CN is the following

$$P_0(\sigma_f) = \frac{1}{2}\int\limits_{\xi_c^{min}}^{\xi_c^{max}} g(\xi_c)\Big[1 - \mathrm{erf}\Big(\frac{\xi_c - \sigma_f}{\sqrt{2}D_{\xi_{11}}}\Big)\Big]\,d\xi_c \tag{2.8}$$

where $g(\xi_c)$ is the density distribution function for critical micro-stresses $\xi_c$

$$g(\xi_c) = \frac{2}{k_{Ic}}\int\limits_{\eta_{min}}^{\eta_{max}} g(\eta)\Big[\int\limits_{\theta_{min}}^{\theta_{max}} g(\theta)g(a)\frac{\sqrt{a^3}}{\varphi(\theta,\eta)}\,d\theta\Big]\,d\eta \tag{2.9}$$

where

$$a = \frac{k_{Ic}}{[\xi_c/\varphi(\theta,\eta)] + \overline{\xi}} \tag{2.10}$$

$g(\theta)$, $g(\eta)$ and $g(A)$ are the density distribution functions for the orientation angles $\theta$, parameter of micro-stress state mode $\eta$ and CN sizes $a^2$, respectively.

The function $g(\eta)$ is determined based on the condition that $\xi_{11}$ and $\xi_{22}$ are distributed by a normal law with variances $(2.1)_{1,2}$.

According to the "weakest link" concept, cleavage fracture of a metal volume $V_I$ occurs if not less than one crack of all numbers of cracks $N_a$ $(N_a = \rho V)$ becomes unstable

$$P(\sigma_f) = 1 - [1 - P_0(\sigma_f)]^{\rho V} \tag{2.11}$$

where $P(\sigma_f)$ is the probability of fracture of macroscopic volume $V$ at uniform distribution of macro-stresses $\sigma_f$.

For inhomogeneous distribution of stresses and strains ahead the crack tip or notch, the expression for probability of global fracture is

$$P(\sigma_f) = 1 - \prod_{i=1}^{i=M} [1 - P_i(\sigma_f)] \tag{2.12}$$

where $P_i(\sigma_f)$ is the probability of metal fracture in $i$-th finite element (FE) volume; $M$ is the number of FE in the "process zone".

In conventional versions of LA, the Weibull distribution is employed instead of expression (2.11) for fracture probability $P_i(\sigma_f)$. In Kotrechko *et al.* (2001) within the framework of the approach proposed, it was shown that the distribution of probability of instability of *one* CN, $P_0(\sigma_f)$ may be approximated by an exponential law. In this case, expression (2.11) may be presented as follows

$$P(\sigma_f) \approx 1 - \exp\Big[-\rho V\Big(\frac{\sigma - \sigma_{th}}{\sigma_u}\Big)^m\Big] \tag{2.13}$$

where $\sigma_{th}$ is the value of threshold stress; $\sigma_u$ is the scale stress; $m$ is the shape parameter of the Weibull distribution.

## 3. Crack nucleation

Prediction of a number of micro-cracks nucleating during plastic deformation is one of the most difficult and less investigated problems of LA. In classic models, determination of length of forming micro-cracks and critical stress of their instability is accentuated. However, as it follows from (2.11) and (2.13), the number of CN significantly influences the value of fracture probability and critical local stress $\sigma_f$. Besides, in most models, the main peculiarity of CN behaviour in metals is not accounted. It is the fact that only freshly nucleated micro-cracks may result in global fracture of the metal. If at the moment of crack nucleation, Griffith's condition for it is not hold, then this crack blunts and now can not "compete" with "fresh" sharp crack nuclei, which is permanently generated during the plastic deformation. This specific feature CN behaviour in a metal was taken into account in the statistical model of fracture proposed in Kotrechko (1995) and multi-scale version of LA developed based on this model (Kotrechko and Meshkov, 2001; Kotrechko, 2002, 2003). In Bordet *et al.* (2005) it was noted that supposition of conventional LA about keeping of the CN activity over the entire loading history is invalid for metals. Therefore, the composition $\rho V$ in (2.11) and (2.13) is not the totality of CN accumulated in the metal during its loading before a certain value of plastic strain $\overline{e}$ is reached, but it is the number of CN, which *arises* at that strain. It means that $\rho$ is the rate of CN generation with respect to strain.

[2]If fracture is initiated by carbide cracking, $g(a)$ is the density distribution function for these particles.

Inhomogeneity of micro-plastic deformation, which gives rise to plastic deformation incompatibility on grain and interphase boundaries, is a general reason for the CN formation in polycrystalline solids. So, in Kotrechko (1995), a statistical model was offered where the formation of CN was considered as a stochastic process of reaching the critical micro-plastic strain value. This model describes the CN formation on micro-scale in terms of average strains over the grain. However, this may be described more thoroughly if one accounts that the local incompatibility of plastic deformations on the grain and interphase boundaries may be described with sufficient accuracy by dislocation pile-ups. The crack nucleus arises if two conditions are held, namely: (i) relaxation in the pile-up tip is absent (pile-up blocking); (ii) formation of the pile-up of critical capacity at which the value of local stresses ahead of its tip is sufficient for formation of atomically sharp flaw near the grain boundary or interphase "ferrite-carbide" boundary[3]. As it is exhibited in Kotrechko *et al.* (2011), formation of such a pile-up may be described as follows

$$CL\Big[\overline{\sigma}(k_\sigma T - M) + \beta\sqrt{\frac{\overline{e}}{d}}\Big]^2 \geqslant \tau_c \tag{3.1}$$

where $C$ is a constant depending on elastic constants of the lattice (for $\alpha$-Fe $C = 0.0336\,\mathrm{N/m}$); $\beta$ is constant ($\beta \approx 2.57\,\mathrm{MPa}\sqrt{\mathrm{m}}$; $d$ is the average grain size; $L$ is the pile-up length; $\overline{\sigma}$ and $\overline{e}$ are equivalent macroscopic stresses and plastic strains, respectively; $k_\sigma$ is a coefficient ($k_\sigma = \sqrt{D_{\xi_{ns}}/\overline{\sigma}}$), where $D_{\xi_{ns}}$ is the variance of shear microscopic stresses $\xi_{ns}$ in the slip systems, (for $\alpha$-Fe and slip systems $\{110\}\langle 111\rangle k_\sigma = 0.225$); $t$ is the dimensionless value of shear stresses $\xi_{ns}$ "applied" to the pile-up ($t = \xi_{ns}/\sqrt{D_{\xi_{ns}}}$); $M$ is the factor averaged over the grain orientation (for b.c.c. crystals $M = 0.36$); $\tau_c$ is the critical shear stress for crack nucleus formation.

In dependence (3.1), the expression $\beta\sqrt{\overline{e}/d}$ specifies the value of shear micro-stresses caused by the interaction of grain of averaged orientation $M$ with plastically deformed to strain $\overline{e}$ surrounding matrix. The value of fluctuation of stresses in the slip system where a pile-up has formed $\xi_{ns}$ is specified by the expression $\overline{\sigma}(k_\sigma t - M)$.

It should be noted that the expression $\beta\sqrt{\overline{e}/d}$ characterizes *shear* micro-stresses induced by dislocations in contrast to $\overline{\xi}$ (Eq. (2.3)), which specifies the *normal* component of the tensor of these stresses. Besides, while determining the value of coefficient $\beta$, a different law for averaging stresses over the pile-up length is used. Accurate to coefficients, the decrease in these stresses at a strain $\overline{e}$ greater than the critical one $e_c$ is described by the same dependence (2.4).

The condition of the pile-up blocking is formulated as follows

$$\sqrt{\frac{L}{r}}\Big[\overline{\sigma}(k_\sigma t - M) + \beta\sqrt{\frac{\overline{e}}{d}}\Big] \leqslant m\tau_Y \tag{3.2}$$

where $r$ is the distance from the grain boundary to the dislocation source in the neighbouring grain ($r \ll L$), where the starting of a such source is possible at reaching the critical value of shear stresses The parameter $m$ characterizes the influence of the slip system orientation of the dislocation source on the value of shear stress acting in this system.

If the fluctuations of values $\tau_Y$ and $r$ are neglected, then the expression for probability of CN formation is the following

$$P_{nucl} = 2\int\limits_{t_c}^{t_{max}} g(t)\Big[\int\limits_{m}^{m_{max}} g(m)\,dm\Big]\,dt \tag{3.3}$$

[3]At certain shape of the carbide particle, carbide cracking is more preferable than CN formation on the interphase boundary.

where

$$m = \frac{\tau_Y \sqrt{\frac{r}{L}}}{\overline{\sigma}(k_\sigma t - M) + \beta\sqrt{\frac{\overline{e}}{d}}} \tag{3.4}$$

The distribution density function $g(m)$ is determined based on the distribution of a scalar angle of misorientation of grain boundaries (Lindley *et al.*, 1970)[4].

According to (3.1), an expression for the critical value $t_c$ is described by the dependence

$$t_c = \frac{1}{k_\sigma}\Big[M + \frac{1}{\overline{\sigma}}\Big(\sqrt{\frac{\tau_c}{CL}} - \beta\sqrt{\frac{\overline{e}}{d}}\Big)\Big] \tag{3.5}$$

The density distribution function $g(t)$ is determined as

$$g(t) = \frac{1}{\sqrt{2\pi}}\exp\Big(\frac{t^2}{2}\Big) \tag{3.6}$$

In some cases, during calculations, it is reasonably to use an approximate expression for $P_{nucl}$. It may be obtained if $m$ fluctuation is neglected. In this case

$$P_{nucl} \approx P(t_c < t < t_r) = 2\int\limits_{t_c}^{t_r} g(t)\;dt \tag{3.7}$$

Accounting for (3.6), $P_{nucl}$ is the following

$$P_{nucl} \approx 2[\varPhi(t_r) - \varPhi(t_c)] \tag{3.8}$$

where $\varPhi(t_r)$ and $\varPhi(t_c)$ are values of the Laplace function at the corresponding value of the parameter $t$.

The expression for the parameter $t_r$ that characterises relaxation conditions is the following

$$t_r = \frac{1}{k_\sigma}\Big[M + \frac{1}{\overline{\sigma}}\Big(\tau_Y m\sqrt{\frac{r}{L}} - \beta\sqrt{\frac{\overline{e}}{d}}\Big)\Big] \tag{3.9}$$

In a general case, the rate of CN generation in the metal volume unit may be specified as

$$\rho = k_\rho P_{nucl} \tag{3.10}$$

where $k_\rho$ is the coefficient depending on the density of carbide particles and grain size. The value of this coefficient may be estimated using an experimental evidence by a calibration procedure.

The approach proposed enables one to model the effect of many factors on the rate of CN generation, such as *metallurgical* factors (average grain size $d$ and maximum grain size $L \approx (0.5\text{-}1.0)d_{max}$), *loading* condition (temperature and loading rate (parameters $\tau_Y$ and $\overline{\sigma}$), *crystallographic texture* (function $g(m)$), the value of *plastic strain* $\overline{e}$. Figure 2 presents the dependence of $\rho$ on the value of plastic strain at different test temperatures for the reactor pressure vessel steel 2Cr-Ni-Mo-V. The specific feature of these dependences is a non-monotonic change of $\rho$ with $\overline{e}$ growth. This agrees well with data of the work by Lindley *et al.* (1970) demonstrating that the number of cleaved carbides grows up to a certain level, after which the nucleation rate decreases monotonically. It should be noted that comparison of the experimental evidence with the obtained results requires to account that $\rho$ is not a *cumulative* CN density, but is the *rate* of its nucleation with respect to strain. Therefore, description of the CN formation on submicroscales enables one to solve adequately one of the key problems of LA related to the prediction of crack formation under the action of plastic flow.

[4]Expression for $g(m)$ is somewhat intricate, so it is not presented in an explicit form.

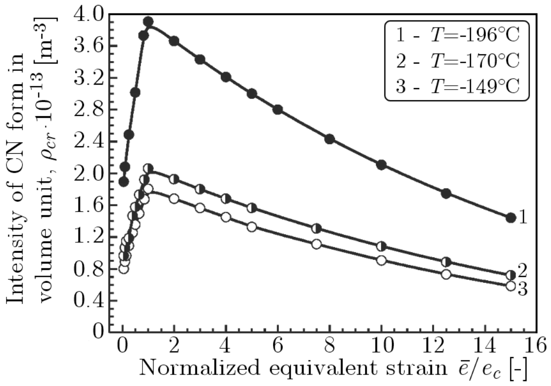


Fig. 2. Dependence of the CN density in RPV steel $\rho$ on the value of plastic strain and temperature: $\overline{e}$ and $e_c$ are the equivalent plastic strain and its critical value, respectively

## 4. Threshold fracture stress

As it is known, the assessment of the threshold stress value is one of the important problems of LA. In most cases, to simplify the calibration procedure, two-parameter Weibull's distribution is employed (Pineau, 2006; Pineau and Benoot, 2010; Beremin, 1983), i.e. it is supposed that $\sigma_{th} = 0$. However, for steels, the value of $\sigma_{th}$ is rather high, and may amount to $\sigma_{th} \approx (0.4\text{-}0.6)\sigma_f$, where $\sigma_f$ is the local fracture stress. So, neglecting the $\sigma_{th}$ value, gives rise to essential errors at the estimation of the Weibull modulus $m$ by experimental evidence. This results in errors of the prediction of scatter and temperature dependence of the fracture toughness. Attempts are known to estimate the value $\sigma_{th}$ by the yield stress at low temperatures. However, it contradicts the physical essence of the threshold fracture stress. According to the model proposed, the value $\sigma_{th}$ may be specified as

$$\sigma_{th} = \frac{\xi_c^{min}}{1 + 3I_{\xi_{11}}} \tag{4.1}$$

where $I_{\xi_{11}}$ is the coefficient of variation of principal tensile micro-stresses $\xi_{11}$ (for ferritic steels under uniaxial tension $I_{\xi_{11}} \approx 0.13$); coefficient "3" means that $\sigma_{th}$ is estimated with probability 0.997; $\xi_c^{min}$ is the minimum value of the critical stress of the CN instability.

According to (2.5)

$$\xi_c^{min} = \Big(\frac{k_{Ic}}{\sqrt{a_{max}}} - \overline{\xi}_{max}\Big)\varphi_{min}(\theta,\eta) \tag{4.2}$$

where $a_{max}$, $\overline{\xi}_{max}$ and $\varphi_{min}(\theta,\eta)$ are the maximum and minimum values of corresponding parameters in dependence (2.5)[5].

Figure 3 illustrates the idea of experimental determination of the value of threshold stress $\sigma_{th}$. According to these data, in the case of uniform distribution of stresses, the average value of fracture stress tends to $\sigma_{th}$ very fastly with an increase in the specimen volume. It enables one to estimate values of $\sigma_{th}$ by the minimum value of brittle fracture stress $R_{MC}$ for standard ($V = 1000\,\text{mm}^3$) tensile specimens over the ductile-to-brittle transition temperature range (Fig. 4) (Kotrechko and Meshkov, 2001)

$$\sigma_{th} = \lambda R_{MC} \tag{4.3}$$

where $\lambda$ is the coefficient whose value depends on the rate of CN generation under the action of plastic deformation. For typical structural steels $\lambda \approx 0.75,\dots,0.95$.

[5] In the first approximation $\varphi_{min}(\theta,\eta) \approx 1$.

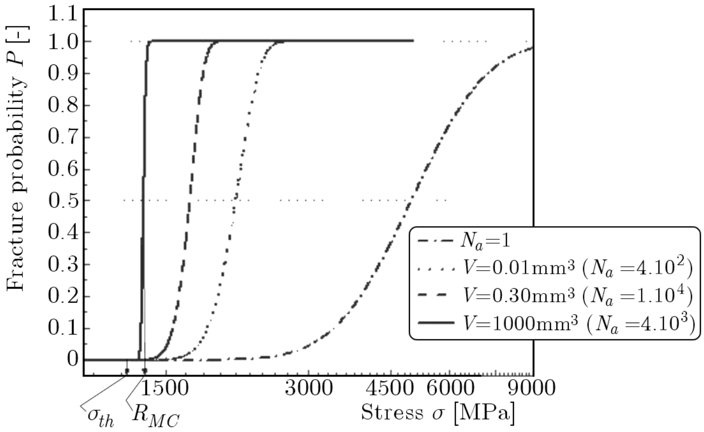


Fig. 3. Dependence of the fracture probability on stress at different volumes $V$ of specimens for RPV steel: $N_a$ is the number of forming CN; $\sigma_{th}$ is the threshold stress; $R_{MC}$ is the minimum level of brittle strength of the standard $(V = 1000\,\mathrm{mm}^3)$ tensile specimen

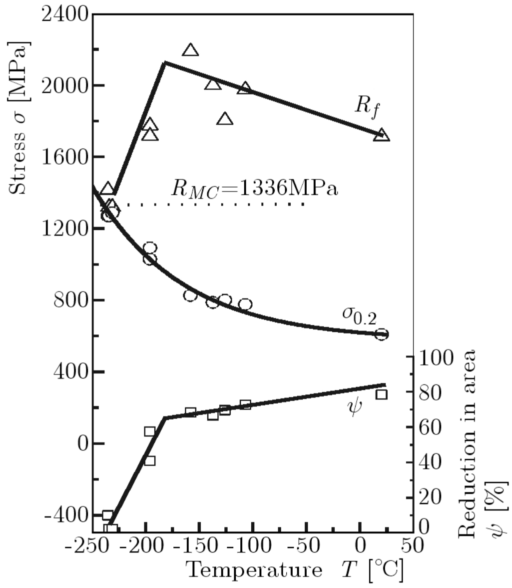


Fig. 4. Temperature dependence of mechanical properties of RPV steel at uniaxial tension: $\sigma_{0.2}$ is the proof stress; $R_f$ is the true fracture stress; $R_{MC}$ is the brittle strength; $\psi$ is the reduction in area

The ductile-to-brittle transition temperature range of high-ductile structural steels for tensile specimens is located below the temperature of boiling of liquid nitrogen $(T = -196°\mathrm{C})$. In this case, $R_{MC}$ value may be determined by the results of tests of cylindrical specimens with notch radius 2 mm at $T = -196°\mathrm{C}$. The use of this technique for $\sigma_{th}$ determination enables one to employ three-parameter Weibull distribution in LA and to improve predictive capabilities of LA.

## 5. Local fracture stress

Initially, LA was aimed at the prediction of a temperature dependence of fracture toughness of steel. However, further development of this approach on the ground of multi-scale models has enabled not only improvement of predictive capabilities of the approach, but also clarificatiob of specific features of the mechanism of cleavage fracture initiation in a highly inhomogeneous stress-strain field ahead the crack tip. Specifically, it appears in the possibility of differentiating the effects both of metallurgical factors and loading conditions (temperature, constraint lost effect etc.) on the fracture limit of structures. The CN instability is the reason for brittle fracture, so the effect of these defects on the local fracture stress is determined through both properties of separate CN (CN length and orientation) and the rate of CN generation during plastic deformation. In terms of the "weakest link" concept, properties of one separate CN predetermine the type and parameters of the function $P_0(\sigma_f)$ in (2.11), and, respectively, the values of Weibull distribution parameters $\sigma_{th}$, $\sigma_u$ and $m$ in dependence (2.13). The effect of the rate of CN generation with respect to strain is characterised by the term $\rho$ in expressions (2.11) and (2.13).

Dependences of the Weibull distribution parameters on the most probable value of the grain size at different magnitudes of grain structure inhomogeneity were obtained in Kotrechko *et al.* (2001). It was exhibited that the values of $\sigma_{th}$ and $\sigma_u$ rise linearly with growth of $1/\sqrt{d_{mpv}}$ ($d_{mpv}$ is the most probable grain size). The value of shape parameter $m$ is virtually independent of $d_{mpv}$, however, it decreases with an increase in the variance of the grain size logarithm $D_{\ln d}$

$$m = a_1 - b_1\sqrt{D_{\ln d}} \tag{5.1}$$

where for iron: $a_1 = 3.35 \pm 0.27$, $b_1 = 1.84 \pm 0.11$.

At the same time, the absolute value of parameter $m$ decreases from 3.0 to 2.1 for typical range of $\sqrt{D_{\ln d}}$ ($\sqrt{D_{\ln d}} = 0.2$-$0.7$).

The normalised value of scaling stress $\sigma_u/\sigma_{th}$ does not depend on the absolute grain size either, and it is a linear function of the variance of grain size logarithms $D_{\ln d}$

$$\frac{\sigma_u}{\sigma_{th}} = a_2 + b_2 D_{\ln d} \tag{5.2}$$

where for iron: $a_2 = 3.81 \pm 0.07$, $b_2 = 11.97 \pm 0.02$ at $\overline{e} = 0.02$.

Their sense is that the parameters of distribution of grain sizes or carbide particles predetermine the distribution of CN lengths. The values of coefficients $a_2$ and $b_2$ depend on the magnitudes of equivalent strain $\overline{e}$. This is due to the effect of dislocation stresses on the value of critical stress of the CN instability $\xi_c$ (Eqs. (2.3)-(2.5)). These dependences are obtained for polycrystalline iron; however, they are correct also for the case of fracture initiation by carbide cracking.

As it was mentioned above, the number $N$ of CN forming at the given value of plastic strain (term $\rho V$ in (2.11) and (2.13)) is the second important factor affecting the local fracture stress $\sigma_f$. As it is shown in Fig. 3, an increase in $N$ gives rise to a decrease in both the average fracture stress and its scatter. This is just the physical nature of the statistical scale effect at cleavage fracture of metals and alloys.

It should be remarked that in the conventional version of LA, the CN density is characterised by the expression $1/V_0$ (where $V_0$ is the reference volume). In the calibration procedure, this value is supposed to be constant. It is one of the reasons for $\sigma_u$ and $m$ dependence on test temperature and notch parameters. Figure 5 presents the dependence $\sigma_f(N_a)$ for uniform stress distribution in an explicit form. According to this evidence, an essential excess of $\sigma_f$ over the brittle strength $R_{MC}$ of standard ($V = 1000\,\text{mm}^3$, $\overline{e} = 0.02$) tensile specimens is observed at $N \geqslant 50000$. At these $N$ values, scatter limits of fracture stress increase significantly. The magnitude of local fracture stress of a metal also depends on the plastic strain value (Fig. 6). This is due to: (i) the effect of dislocation micro-stresses $\overline{\xi}$ on the instability of separate CN, and (ii) dependence of their rate creation on the value of plastic strain (Fig. 2). It should be noticed that in the existing versions of LA, the attempts were made to account for this effect by the introduction of phenomenological dependences of the Weibull stress $\sigma_W$ on the strain value (Bordet *et al.*, 2005; Beremin, 1983). Dependences in Fig. 5 are obtained for the case of uniform stress and strain distribution (solid and dash lines). In the vicinity of a macro-crack or notch, these distributions are essentially non-uniform. This gives rise to difficulties in the

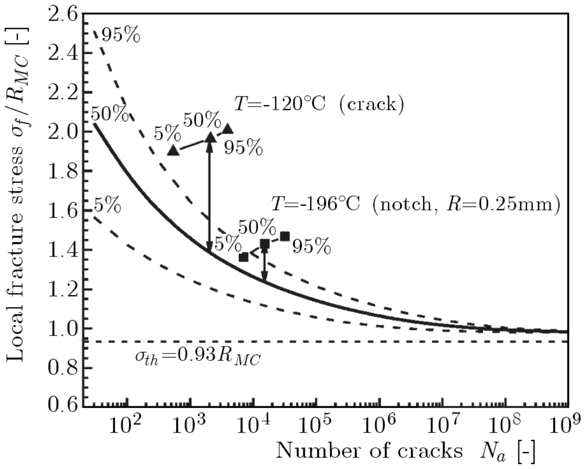


Fig. 5. Dependence of the normalized value of fracture stress $\sigma_f$ on the CN number $N$ for fracture probabilities 5%, 50% and 95% at $T = -196$°C under uniform uniaxial tension; (▲, ■ are values of the local fracture stress $\sigma_f$ ahead the macro-crack or notch of $R = 0.25$ mm at the corresponding values of fracture probability (the arrows indicate the effect of local plastic strain gradient)

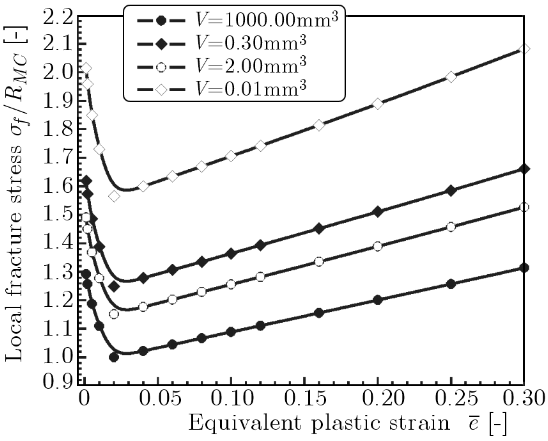


Fig. 6. The effect of plastic strain on the value local fracture stress $\sigma_f$ for different volumes of the plastically deformed metal

determination of the local fracture stress value. In the conventional Beremin version of LA, the Weibull stress $\sigma_W$ is used as a measure of local stress. This stress is an integral characteristic of brittle strength for the region subjected to local yielding. Another approach to this problem was offered in Lin *et al.* (1986) and developed in Kotrechko and Meshkov (2001), Kotrechko (2002). In this case, the local fracture stress $\sigma_f$ is determined as the value of tensile stress $\sigma_{11}$ in the locus where the probability of fracture initiation reaches it maximum value (Fig. 7). Such an approach enables one to compare directly the calculated magnitude $\sigma_f$ with the experimental evidence determined by the value of tensile stresses at the cleavage initiation site ahead of the macro-crack tip. Besides, it permits one to ascertain the region where fracture initiates ("process zone") (Fig. 7). As it is exhibited in Kotrechko and Meshkov (2001, Kotrechko (2003), this area is much less than the whole region of local plastic yielding.

According to the computer simulation findings on fracture of the reactor pressure vessel steel, in addition to the CN number, the value of stress-strain field inhomogeneity ahead the macro-crack influences the value of local fracture stress $\sigma_f$ (Fig. 5). This effect depends on CN density. The smaller the density of forming CN, the stronger the effect of strain gradient on the value of $\sigma_f$. The higher the stress value $\sigma_f$, the higher the fracture toughness $K_{Ic}$, so

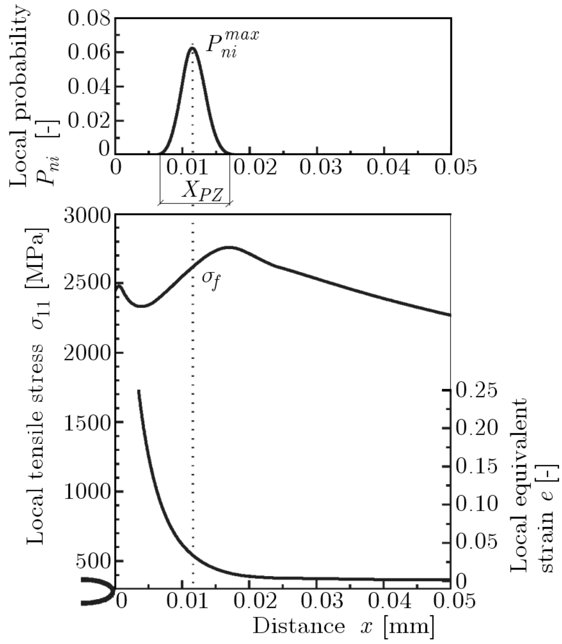


Fig. 7. Distribution of local tensile stresses $\sigma_{11}$, equivalent local plastic strain $\overline{e}$, and local probability $P_{ni}$ of fracture initiation ahead the crack tip in the pre-cracked Charpy surveillance specimen at temperature $-120°$, $K_{Jc} = 59.4\,\mathrm{MPa}\sqrt{\mathrm{m}}$ and the probability of global fracture $P_\Sigma = 0.63$; $X_{PZ}$ is the size of the "process zone" in the minimum cross-section of the specimen

manufacturing of steels with a low rate of CN generation will significantly increase their fracture toughness and decrease their sensibility to crack-like defects. The latter is especially important for high-strength steels.

## 6. Multiple-barrier effect

Ascertainment of the critical event of micro-crack growth, which governs the global fracture, is one of urgent problems of LA (Pineau and Benoot, 2010). The simplest model that enables one to estimate the critical size of carbide micro-crack, which instability gives rise to global fracture, was offered by Martin-Meizoso *et al.* (1994)

$$\frac{a}{d} \leqslant \left(\frac{k_{Ia}^{c/f}}{k_{Ia}^{f/f}}\right)^2 \tag{6.1}$$

where $d$ is the ferrite grain size; $k_{Ia}^{c/f}$ and $k_{Ia}^{f/f}$ are the critical values of stress intensity coefficient corresponding to overcoming the interphase boundary "carbide-ferrite" and the ferrite grain boundary, respectively. The value of $k_{Ia}^{c/f}/k_{Ia}^{f/f}$ must be less than $\sim 1/5$. It means that unstable propagation of the carbide crack will give rise to global fracture if its size is at least 25 times less than the grain size. For typical steels, this condition is usually held. However, a great number of arrested cleavage micro-cracks is observed in steels, see for example Lambert-Perlade *et al.* (2004). This is due to three main factors: (i) random size of carbide particles and grains; (ii) statistic distribution of ferrite grain boundary misorientations; (iii) fluctuation of tensile micro-stresses which changes from grain to grain. In Kotrechko (1995) an approach was formulated that enables modelling of micro-crack propagation in the polycrystalline aggregate accounting for these factors. Within the framework of such an approach, an expression for the critical value of micro-stresses $\xi_c^L$ required to support the unstable propagation of a crack of length $L$, is the following

$$\xi_c^L = \frac{2}{\pi L}\Big(\int_0^{d_c} \xi_c^d \sqrt{\frac{x}{L-x}}\, dx + \int_d^{2d} \xi_c^{2d} \sqrt{\frac{x}{L-x}}\, dx\Big) \tag{6.2}$$

where $\xi_c^d$ is the critical level of tensile stresses in the first grain, which guarantees its cleavage (Fig. 9); $\xi_c^{2d}$ is the critical cleavage stress for the second grain.

The value of critical stress required for cleavage of the first grain and overcoming the grain boundary may be specified as

$$\xi_c^d = \alpha \xi_c \tag{6.3}$$

where

$$\alpha = \sqrt{\frac{a}{d}} \frac{k_{Ia}^{f/f}}{k_{Ia}^{c/f}} \tag{6.4}$$

The probability of cleavage of grain #1 (Fig. 8) resulting in formation of a disk-like crack of diameter $L = d$ at the given level of *macro-stresses* $\sigma_f$ is described by the dependence

$$P_2(\sigma_f) = \int_{\xi^d_{c\,min}}^{\xi^d_{c\,max}} g(\xi_c^d) P_1(\sigma_f|\xi_c^d)\, d\xi_c^D \tag{6.5}$$

where $g(\xi_c^d)$ is the distribution density function determined by (2.9) accounting for conditions (6.3); $P_1(\sigma_f|\xi_c^d)$ is the conditional probability

$$P_1(\sigma_1|\xi_c^d) = \frac{1}{\sqrt{2\pi D_{\xi_{11}}}} \int_{\xi_c^d}^{\xi_{11}^{max}} \exp\Big(\frac{\xi_{11}-\sigma_f}{\sqrt{2D_{\xi_{11}}}}\Big)\, d\xi_{11} \tag{6.6}$$

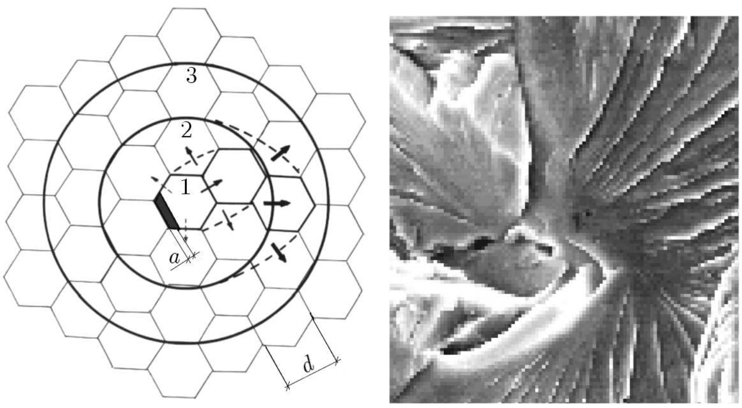


Fig. 8. Scheme of micro-crack growth in a polycrystalline metal: $a$ is the initial CN size; $d$ is the grain size; 1, 2, 3 are numbers of disk-like cracks at different steps of their extension

As it is shown in Fig. 8a, the further stage of formed disk-like crack #1 is the transition to not less than one of $m$ neighbouring grains (at this step of the crack growth $m = 6$). This gives rise to formation of disk-like crack #2. For this event, the value of probability is following

$$P_4(\sigma_f) = \int_{\xi^d_{c\,min}}^{\xi^d_{c\,max}} \int_{\xi^{2d}_{c\,min}}^{\xi^{2d}_{c\,max}} g(\xi_c^d, \xi_c^{2d}) P_3(\sigma_f|\xi_c^d, \xi_c^{2d})\, d\xi_c^d\, d\xi_c^{2d} \tag{6.7}$$

Disk-like crack #3 and the further ones are formed similarly.

If the fluctuation of the coefficient $\alpha$ in (6.4) is neglected, then dependence (6.7) will simplify to

$$P_4(\sigma_f) = \int\limits_{\xi^d_{c\,min}}^{\xi^d_{c\,max}} g(\xi^d_c) P_3(\sigma_f|\xi^d_c, \xi^{2d}_c)\, d\xi^d_c \tag{6.8}$$

where

$$P_3(\sigma_f|\xi^d_c, \xi^{2d}_c) = 1 - [1 - P(\xi_{11} > \xi^D_c, \xi^{2D}_{11} > \xi^{2D}_c)]^m \tag{6.9}$$

Therefore, the crack growth in a polycrystalline metal consists in realisation of two sequentially repeating events related to cleavage of not less than one grain neighbouring to the disk-like crack with consequent formation of the disk-like crack with a greater diameter. Such a mechanism is similar to the dislocation kink moving. The difference is that the dislocation kink is created by thermal fluctuations, and in the crack movement it is due to fluctuation of tensile micro-stresses $\xi_{11}$ and stochastic misorientation of grain boundaries. The fanlike type of the cleavage initiation site is one of the consequences of such a micromechanism (Fig. 8b). Figure 9 shows computer simulation findings on crack growth in polycrystalline iron with a average grain size $97\,\mu$m and the variance of grain logarithms $D_{\ln d} = 0.19$. This simulation was executed for an *extremely unfavourable* condition $\alpha = 1$ for overcoming the grain boundary by the crack. According to the data obtained, in the case $\alpha = 1$[6], the level of average critical macro- stress of unstable propagation of carbide crack within the grain $\sigma_f$ is sufficient for further growth of this crack on macroscopic scale. It should be noted that this is a dependence for *average* macroscopic fracture stress. As it follows from the suggested model, some cracks are arrested due to micro-stress $\xi_{11}$ fluctuations and grain boundaries. This gives rise to presence of arrested cracks with a size equal to 1-2 grain sizes in the fractured specimens.

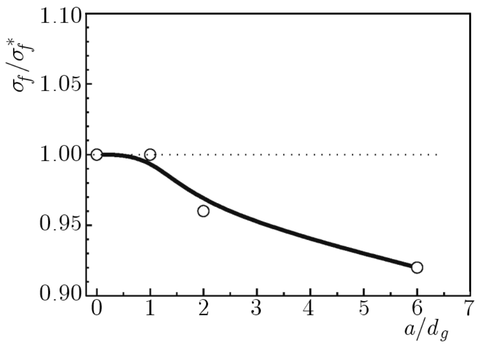


Fig. 9. Change in the average value of stress of micro-crack instability $\sigma_f$ on its diameter $a$: $\sigma_f^*$ is the critical stress of overcoming the grain boundary (of grain cleavage); $d_g$ is the average grain size

## 7. Conclusions

- The multi-scale approach to fracture enables one to overcome several essential challenges of the conventional Local Approach:
  - to offer a statistica criterion of cleavage fracture initiation accounting for fluctuation of micro-stresses;

[6]It means that at $d/a = 100$, the ratio $k^{f/f}_{Ia}$ and $k^{c/f}_{Ia}$ reaches an extremely high level equal to 10.

– to propose a dependence describing the effect of plastic strain, temperature and loading rate on the crack nuclei generation rate;
– to differentiate contribution of properties of a separate crack nucleus and the rate of crack nuclei generation to change in the value of local fracture stress $\sigma_f$ and fracture toughness.

- The value of shape parameter of the Weibull distribution for one crack nucleus instability $m$ does not depend on the grain/carbide particle size; however, it is a linearly decreasing function of square root from logarithm of this size variance $\sqrt{D_{\ln d}}$.
- The normalized value of the scaling stress $\sigma_u/\sigma_{th}$ is a linear function of $\sqrt{D_{\ln d}}$.
- The dependence of the value of critical cleavage stress on the number of forming crack nuclei is the reason for the statistical scale effect at cleavage fracture of metals. For $\alpha$-Fe and steels, this effect becomes quantitatively essential only for extremely small volumes $V \leqslant 0.1\,\text{mm}^3$, and may amount to double increase for $V \leqslant 0.001\,\text{mm}^3$. Such small volumes limit the "process zone" ahead the sharp cracks.
- The gradient of local plastic strain is one of the factors affecting the value of local fracture stress $\sigma_f$. Reduction in the crack nuclei density gives rise to an increase in the susceptibility of $\sigma_f$ to the magnitude of the gradient value.
- A relation exists between the value of threshold stress of cleavage fracture $\sigma_{th}$ and the minimum fracture stress of standard tensile specimens $R_{MC}$, namely $\sigma_{th} = (0.75\text{-}0.95)R_{MC}$. This enables one to suggest a simple procedure of $\sigma_{th}$ determination in the Local Approach to fracture.
- The mechanism of micro-crack propagation in polycrystalline metals consists in realization of two sequentially repeating steps related to cleavage of not less than one grain neighbouring to the disk-like crack with further crack growth in the tangential direction resulting in formation of the disk-like crack with a greater diameter.

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## Kluczowe zagadnienia w lokalnym ujęciu kruchego pękania

Streszczenie

W oparciu o zaproponowany wieloskalowy model lokalnego sformułowania procesu pękania (*Local Approach* – LA) wyróżniono cztery podstawowe problemy do rozważenia: (i) efekt fluktuacji mikronaprężeń na niestabilność jądra pęknięcia, (ii) intensywność zawiązywania się mikropęknięcia i jego wpływ na prawdopodobieństwo powstania przełomu, (iii) teoretyczne i eksperymentalne oszacowanie wartości naprężenia krytycznego, (iv) stochastyczna analiza efektu „wieloprogowego” na wzrost mikropęknięcia w metalu polikrystalicznym.

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