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Local approach and FEM in brittle fracture prediction

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Local approach in fracture mechanics is based on the application of appropriate failure micromechanistic models to make predictions of fracture behaviour. The FEA of crack-tip and an associated post-processing routine is usually applied. Here should be noted the distinction between the cells of material, having characteristic microstructural dimensions, which constitute the cleavage process zone, and the corresponding finite elements used to represent their behaviour. Predictions of brittle fracture are based on the Beremin local approach model, where the Weibull location parameter σ_u and shape parameter m have been calculated using FEM for Charpy type specimen. These parameters are considered to be transferable material properties, independent of temperature, specimen geometry or loading mode and can be used for prediction of the stress intensity factor K.

1. Introduction

The main factors influencing the brittle failure initiation is the presence of stress concentrators, temperature and loading rate. In general, assessment of fracture resistance and failure prediction can be based on global or local approach. Global material characteristics (e.g. fracture toughness, K_{IC}, critical value of J_{I} — integral, J_{IC}) are used for the assessment of defect tolerance. Compared to global approach, the local approach takes into account the micromechanism of fracture initiation in the plastic zone ahead of the crack or the notch tip. The knowledge of local material parameters representing the resistance of particular material to failure may be used for the prediction of limit state of notched or cracked bodies, or for the prediction of global fracture characteristics. Within this context, we apply local approach and damage mechanics methodologies to predict the fracture behaviour of low alloyed CrMoV rotor steel. Some microstructures have been tested and two were selected to study their influence on the local parameters. The predictions are illustrated using the Beremin local approach model.

2. Scientific background

At present, the local approach to assessment of failure can be divided into two basic concepts: (i) *Deterministic* — introducing material parameter called as cleavage fracture stress, σ_{CF}, which is macroscopic parameter characterizing the microscopic resistance of the given material to brittle fracture and is associated with the processes of nucleation and propagation of cleavage microcracks. Based on this concept, the initiation of the brittle fracture occurs when local maximum principal stress, $\sigma_{1\max}$, is equal to the cleavage fracture stress, σ_{CF}, [1] or [2]. (ii) *Statistic* concept — it was experimentally proved, that the cleavage fracture stress exhibits large scatter of experimental data for some materials (tempered bainitic steels for example). This scatter in fracture criteria is inherent property of such materials. The main difference between the deterministic and the statistic concept may be seen in the cleavage fracture initiation criterion. While in the former the initiation location is pre-determined by a site of local maximum stress, in the latter the cleavage microcracks are created in a small volume V_o (cell) located in any place in the plastic zone ahead of crack tip (the weakest link model) [3].

There has been imposed considerable effort to study the effect (fracture toughness locus) of brittle fracture initiation parameters (K_{IC} and J_C) on crack length — specimen geometry (Q-constraint indexing parameters) using both approaches. There is still considerable discussion about the most appropriate local parameters, but it was showed that local parameters, σ_u and m are not dependent on crack length and Q parameter [4].

According to Beremin conception [3], the material is modelled as a set of grains having constant volume V_o (recent work [5] mentions chain of cells having characteristic microstructural dimensions) and forming the cleavage process zone. Probability of brittle failure of cell is given by applied stress σ:

$$P_f = (\sigma/\sigma_u)^m. \tag{1}$$

Cumulative probability of failure of generally loaded component can be obtained introducing the Weibull stress into above equation and

$$P_f = 1 - \exp\{-(\sigma_w/\sigma_u)^m\}. \tag{2}$$

The stress σ_w is given [3] by expression

$$\sigma_w = \left\{\sum \sigma_1^m (V_i/V_o)\right\}^{1/m}. \tag{3}$$

V_i is a volume in which the principal stress σ_1 is acting and it is practically determined by the corresponding mesh element used by FEM. The element volume V_i has maximally the same size as the characteristic cell volume V_o. The summation is evaluated only over plastically deformed elements assuming that microcracks are not created in the cells residing outside the crack-tip plastic zone. The characteristic volume V_o (cell size) can be chosen arbitrarily, but small enough to catch micromechanisms which play major role in fracture process. In practice, this defines a minimum size of V_o in the order of about ten grain sizes [6].

A number of micromechanical models for transgranular cleavage fracture have been proposed, most derived from weakest-link statistics. The model for cleavage fracture can be based on the three-parameter Weibull form, e.g.:

$$\sigma_w = \left\{\sum (1 - P^i_{\text{void}})(\sigma^i_1 - \sigma_{\text{th}})^m (V_i/V_o)\right\}^{1/m}, \tag{4}$$

where σ_{th} is a threshold stress and P^i_{void} is the void nucleation probability of V_i [7]. The Roussselier ductile damage model was shown e.g. in [5].

3. Material and experimental procedures

The CrMoV rotor steel having chemical composition (in wt. %): 0.23 C, 0.64 Mn, 0.28 Si, 0.022 P, 0.028 S, 1.23Cr, 0.55 Mo, 0.16 V has been utilized for experiments. Steel was commercially produced, hot rolled bar having section 30 × 60 mm^2. A range of microstructures has been tested to study the upper nose temper embrittlement phenomena and the next two types were selected: (i) ferrite with fine carbides (FC) and (ii) ferrite with coarser carbides (CC).

The yield strength and true stress-strain curves have been measured using cylindrical specimens over temperature range of –196 to 200 °C at cross-head speed of 2 mm·min^{-1}. The yield strength was taken to be the lower yield stress value (R_{eL}) or the 0.2 % proof stress ($R_{p0.2}$). Temperature dependencies on fracture toughness have been measured using 25 mm thick specimen loaded at three point bending at cross head speed of 1 mm·min^{-1}.

Axisymetrically notched tensile specimens with diameter of 16 mm were tested using diametral extensometer for measurement of strain at fracture. The geometry of this notch was comparable with V notch of Charpy type specimen.

For one selected temperature in lower shelf region (below t_{GY}) a range of test was performed to obtain data for statistical treatment. Determination of t_{GY} can be found in [8].

4. Local parameters

Accepting the Beremin approach to the analysis of local criterion for cleavage fracture, the local parameters for Charpy type specimen were calculated using FEM. Tensile characteristics representing both materials used are given in Table 1. The stress strain curves were approximated using bilinear parameters (E and E_t) as shown in Table 1.

Table 1. Data measured experimentally and those used in FEM calculations.

	test temp. [°C]	$R_{p0.2}$ [MPa]	R_m [MPa]	E [MPa]	σ_y [MPa]	E_t [MPa]	ν
FC	-80	868	980	2.05e5	960	1.05e4	0.3
CC	-150	729	846	2.05e5	814	1.10e4	0.3

Finite element package ANSYS 5.1 was used for calculations. The flow behaviour was computed using incremental plasticity. The attention was paid to implementation of the true stress–strain curve. Then the Weibull shape parameter, m, and Weibull stress, σ_w, were determined by integration in the plastic zone ahead of the crack tip for estimated values of characteristic cell V_o. The Weibull parameter m was determined by an iterative process. A linear regression of $\ln[\ln\{1/(1-P_F)\}]$ versus $ln(\sigma_w)$, with P_F at the fracture points taken equal to the rank probability of the fracture points within the series, then results in a slope m^* and σ_u value. This is repeated with an adjusted m value for computing the Weibull stress until the regression slope m^* is equal to the assumed m value. Once the value of m has been determined, the value of σ_u was read from the linear regression for $P_f = 0.63$. Similar procedure was applied for determination of local parameters for notched tensile specimens.

Based on the experimental results generated on nine Charpy V-notch specimens for both FC and CC microstructure, the local parameters, σ_u and m were obtained. The results of calculations for various cell size, V_o, are given in Table 2, the cell size is represented by parameter λ, according to equation $V_o = \lambda^3$. Using parameters given in Table 2 the effects of cumulative probability on Weibull stress σ_w have been plotted for both microstructures investigated (Figs. 1a and 1b).

Table 2. Local parameters calculated for various cell size.

	$\lambda =$	$50\mu m$	$\lambda =$	$75\mu m$	$\lambda =$	$100\mu m$	$\lambda =$	$125\mu m$
	m	σ_u [MPa]	m	σ_u [MPa]	m	σ_u [MPa]	m	σ_u [MPa]
FC	12.52	4500	12.57	4081	12.56	3809	–	–
CC	14.20	3450	–	–	14.38	3015	14.46	2875

Local parameters for CNV bend specimen were compared with results generated for the axisymmetric notched specimens. The tests were carried out at the same temperatures at which the static bend tests of CNV specimen, i.e. at the condition of quite cleavage failure. Small difference of σ_u values obtained from those evaluated by means of Charpy specimens has been found. Nevertheless, the conclusion concerning the intrinsic resistance to cleavage fracture of microstructures investigated is consistent with that resulting from Charpy specimens.

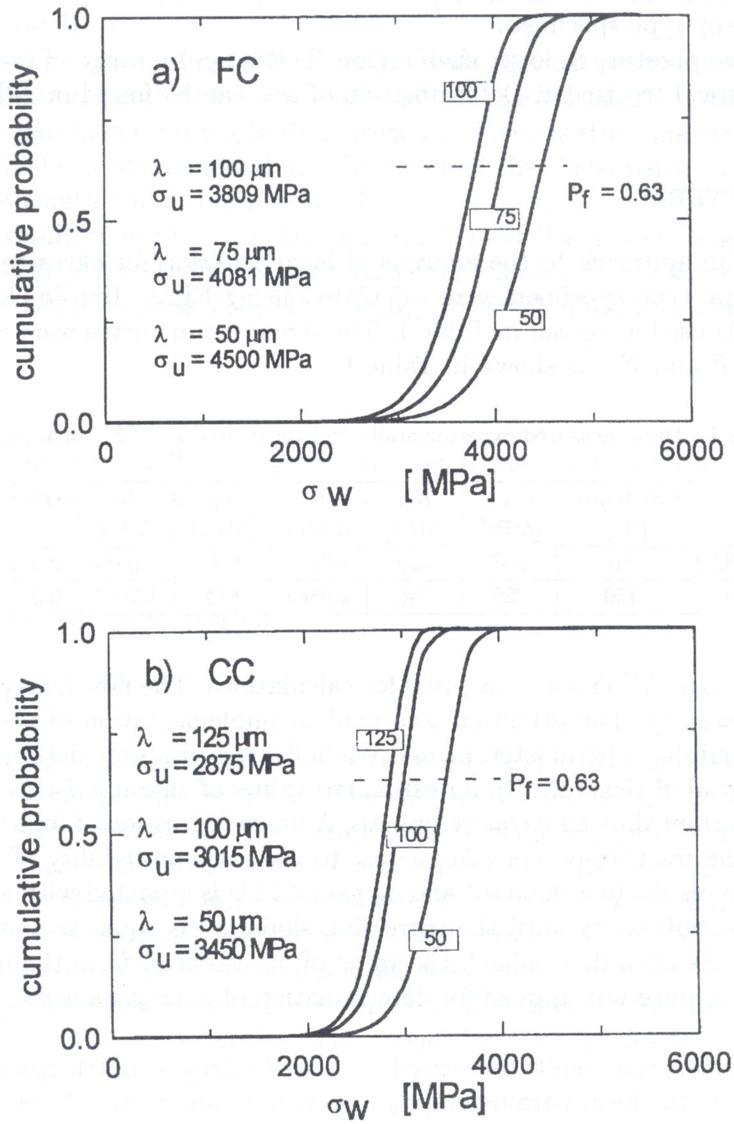

Fig. 1. Cumulative probability of Weibull stress as a function of cell size.

5. Prediction of Fracture Toughness Scatter

In order to test the reliability of determined local parameters the comparison of predicted temperature dependence on fracture toughness with measured data was carried out. For small-scale yielding, the stress intensity factor, K, associated with the given cumulative failure probability, P_f, is given by:

$$K = \{\ln(1/(1 - P_\mathrm{f}))(V_\mathrm{o}\sigma_\mathrm{u}^m/(\sigma_\mathrm{y}^{m-4}BC_\mathrm{m}))\}^{1/4} \tag{5}$$

in [5], where B represents specimen thickness, and C_m is effectively a numerical constant. The values of the constant C_m was obtained as follows. A large strain elastic-plastic analysis of SENB specimen was conducted, and the result plotted as $\ln(\sigma_\mathrm{w}/\sigma_\mathrm{u})^m$ vs. $\ln(J/b\sigma_\mathrm{y})$. The equation 4 was re-arranging into the same form to compare the both curves.

The values of the constants used for K factor prediction were $C_{\mathrm{m}} = 2e3$ (obtained from large-strain elastic-plastic analysis), $V_{\mathrm{o}} = (50\mu\mathrm{m})^3$, and σ_{u} and m are given in Table 2 for both types of microstructures. Figure 2 shows reasonable prediction of toughness behaviour at lower temperatures. This is not surprising, since at higher temperatures the elasto-plastic behaviour is dominating.

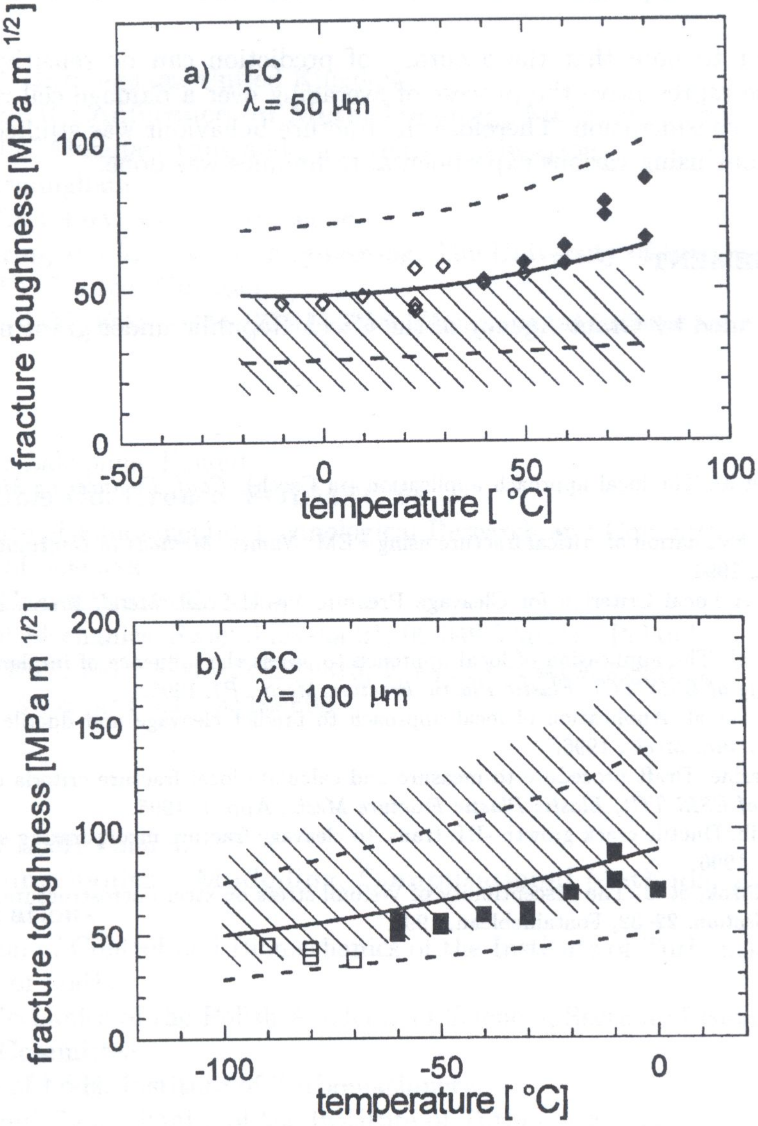

Fig. 2. Prediction of fracture toughness for $P_{\mathrm{f}} = 0.05, 0.5, 0.95$ (full and dashed lines) and for evidently wrong values of λ — in case of FC $\lambda = 100\mu$m, in case of CC $\lambda = 50\mu$m.

6. Conclusion

Accepting the Beremin concept in local approach the local criteria for cleavage fracture were calculated for two different types of microstructures. The ferrite with fine carbides exhibits higher values of stress σ_{u} when compared to the ferrite with coarse carbides. Location parameter σ_{u} was shown to be a strong function of cell size V_{o} chosen. The enhancement of cleavage fracture initiation probability in cell volume corresponds well to carbide induced cleavage due to higher carbide thickness.

The expression for K predicts correctly the temperature dependence on fracture toughness at lower temperatures.

All predictions in this investigation were based on two-dimensional finite element analysis with assumed plane strain behaviour. Although it is believed that the behaviour near the crack tip, which controls the cleavage predictions, is approximated well by assuming plane strain, three dimensional analysis should be performed to verify this. The better results in predictions can be probably received by using a three parameter Weibull models what will be taken into account in some future works.

It is important to note that the accuracy of prediction can be sensitive to the selection of finite element size representive the process of averaging over a damage cell relevant to the failure mechanism under consideration. Therefore the fracture behaviour was studied in detail in [8] and a lot of observations using various experimental techniques was done.

Acknowledgement

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