Application of the Local Approach for Prediction of Ductile Fracture of Highly Irradiated Austenitic Steels

Boris Margolin[1,*], Alexander Sorokin[1], Victor Kostylev[1]

[1] Central Research Institute of Structural Materials "Prometey", Saint-Petersburg, Russia
* Corresponding author: margolin@prometey2.spb.su

Abstract The physical-and-mechanical model of ductile fracture has been developed to predict fracture toughness and fracture strain of irradiated austenitic steels taking into account stress-state triaxiality and irradiation swelling. Comparison of experimental data on fracture strain of irradiated austenitic weld metal with predicted results by the model has been performed. The model also allows to describe sharp decrease of ultimate strength on the basis of the proposed mechanism called as "the running collapse mechanism".

Keywords Ductile fracture model, Fracture toughness, Swelling, Irradiated austenitic steels, Vacancy voids

1. Introduction

Ductile fracture of unirradiated austenitic and ferritic steels may be sufficiently successfully described on the basis of well known model – The Gurson-Tvergaard-Needleman model (GTN-model) [1, 2], and also on the basis less known model – Margolin-Karzov-Shvetsova-Kostylev model (MKSK-model) [3].

Ductile fracture of irradiated austenitic steels has many features. Some of them are the following.
(1) Ductile fracture is controlled by not only evolution of voids, nucleating by deformation (deformation voids), but also by vacancy voids (resulting in swelling) arising under irradiation before deformation.
(2) Deformation voids nucleation rate is higher for irradiated steel than for unirradiated steel.
(3) Neutron irradiation reduces fracture toughness stronger than fracture strain of tensile smooth specimens. It means that stress state triaxiality (SST) enhances the effect of neutron irradiation on fracture strain.
(4) For some value of radiation swelling a fracture of smooth specimens occurs when stress less than yield strength, but fracture surface contains dimples. It means that fracture mechanism is ductile due to evolution of voids.

The aim of this paper is development of MKSK-model for prediction the fracture strain on neutron dose for different stress states, prediction the influence of neutron irradiation and radiation swelling on material fracture toughness and also prediction fracture at high level of swelling when stress less than yield strength.

2. The main considerations of the physical-mechanical ductile fracture model

The main considerations of the proposed model are following:

(a) Fracture proceeds by the mechanism of nucleation, growth and coalescence of voids. Two void populations are considered: vacancy voids and deformation voids, i.e. voids nucleating during the process of material deformation.

(b) Polycrystalline material is presented as an aggregate of unit cells in the form of cubes with homogeneous properties of a material.

(c) The rate of change of void volume concentration $\frac{d\rho_v^{def}}{d\sigma_{nuc}}$ is presented in the form

$$\frac{d\rho_v^{def}}{d\sigma_{nuc}} = \frac{\rho_v^{max} - \rho_v^{def}}{\sigma_d}, \tag{1}$$

where ρ_v^{def} is the concentration of deformation voids in a unit of volume of a material matrix, ρ_v^{max} is the maximum volume concentration of void nucleation sites.

In (Eq. 1) σ_{nuc} is stress which controls nucleation of discontinuity near some barriers [4, 5]. In case of void nucleation the following barriers are considered: inclusions of second phase or coarse carbides and others. According to papers [4, 5] σ_{nuc} can written in the form

$$\sigma_{nuc} = \sigma_1 + m_{T\varepsilon} \cdot \sigma_{eff}, \tag{2}$$

where the parameter $m_{T\varepsilon}$ is concentration coefficient of local stress near dislocation pile-up; σ_1 is maximum principal stresses; $\sigma_{eff} = \sigma_{eq} - \sigma_Y$ is effective stress; σ_{eq} is equivalent stress; σ_d is a local strength of matrix-inclusion interface.

In general case σ_d depends on neutron dose and does not depend on test temperature [4, 5]. It is necessary to note that equation for σ_{nuc} is similar to equation proposed in paper [6].

From (Eq. 2) it follows that as a neutron dose D increases, σ_{nuc} will increase at the expense of an increase of σ_Y and, correspondingly, σ_1. According to papers [4, 5], as a dose D increases, σ_d decreases. Then from (Eq. 1) it follows that irradiation results in an increase of void concentration. This conclusion following from the considered equations is confirmed by the experimental data. It is shown in paper [7] that dimple concentration on a specimen surface in an irradiated condition is higher than that in the initial one.

(d) When analysing the growth of vacancy and deformation voids the Huang's equation [8] is used. To describe a void growth under conditions of their interaction an additional factor was introduced into Huang's equation in the form $\frac{1}{1-f}$

$$\frac{dV_{void}}{V_{void}} = \frac{3 \cdot \alpha}{1-f} \cdot d\text{æ}, \tag{3}$$

where

$$\alpha = 0.427\left(\frac{\sigma_m}{\sigma_{eq}}\right)^k \cdot \exp\left(\frac{3}{2}\frac{\sigma_m}{\sigma_{eq}}\right); \quad k = \begin{cases} 0{,}25, \text{ for } \frac{\sigma_m}{\sigma_{eq}} \le 1 \\ 0, \text{ for } \frac{\sigma_m}{\sigma_{eq}} > 1 \end{cases}; \tag{4}$$

$\text{æ} = \int d\varepsilon_{eq}^p$ is the Odquist's parameter; $d\varepsilon_{eq}^p$ is equivalent of a plastic strain increment, f is material void volume fraction

$$f = \frac{V_\Sigma}{V + V_\Sigma}, \tag{5}$$

In (Eq. 5) V_Σ is the total volume of vacancy and deformation voids in a material matrix of the volume V.

(e) The criterion of a unit cell plastic collapse or, in other words, the criterion of plastic instability is used as fracture criterion [3, 9]

$$\frac{dF_{eq}}{dæ} = 0, \tag{6}$$

where $F_{eq}=\sigma_{eq}\cdot(1-\overline{A}_\Sigma)$, σ_{eq} is equivalent stresses related to a material matrix (without voids), $\overline{A}_\Sigma$ is a relative void area, i.e. void cross-section area related to the cross-section area unit of a unit cell with voids. It should be noted that when analysing conditions in (Eq. 6) stress state triaxiality is taken to be constant [3].

The parameter $\overline{A}_\Sigma$ is calculated on the basis of following considerations. In the general case α in (Eq. 4) depends on æ and does not depend on a void volume. Then an increase in the volume of vacancy and deformation voids taking into account (Eq. 1) and (Eq. 3) may be calculated by the equation:

$$d\overline{V}_\Sigma = \frac{3\cdot\alpha}{1-f}\cdot\overline{V}_\Sigma\cdot dæ + V_{nuc}^{def}\cdot\left[\rho_v^{def}(æ+dæ)-\rho_v^{def}(æ)\right], \tag{7}$$

where V_{nuc}^{def} is the volume of a nucleus deformation void.

When integrating (Eq. 7) the initial condition is formulated in the form:

$$\left(\overline{V}_\Sigma\right)_0 = S_w + V_{nuc}^{def}\cdot\left[\rho_v^{def}(æ=0)\right], \tag{8}$$

where $\left(\overline{V}_\Sigma\right)_0$ is the value of a relative void volume with æ=0, S_w is material swelling.

The parameter $\overline{A}_\Sigma$ is connected with volume of voids by the following manner

$$\overline{A}_\Sigma = \left(\frac{\overline{V}_\Sigma}{1+\overline{V}_\Sigma}\right)^{2/3}. \tag{9}$$

It is necessary to note that for prediction of material behavior in ductile fracture regime GTN-model [1, 2] is widely used. According to this model the plastic potential introduced by Gurson [1] is presented in the form

$$\Phi = \frac{{\sigma_{eq}}^2}{{\sigma_2}^2} + 2f^*q_1\cdot\cosh\left(\frac{3}{2}q_2\frac{\sigma_m}{\sigma_S}\right) - [1-(q_1f^*)^2 = 0, \tag{10}$$

where σ_S is the function describing the yield surface for material without voids, q_1, q_2,f_c and k_a are material constants;

$$f^* = \begin{cases} f & \text{for } f \le f_c \\ f_c + k_a(f-f_c) & \text{for } f > f_c \end{cases}. \tag{11}$$

The increase of void volume fraction is written

$$df = df_{nucl} + df_{growth}, \tag{12}$$

where

$$df_{growth} = (1-f)d\varepsilon_{ii}^p, \tag{13}$$

In (Eq. 13) $d\varepsilon_{ii}^p$ is the sum of normal plastic strain. Value of $\frac{df_{nucl}}{dæ}$ may be calculated by formula [10]

$$\frac{df_{nucl}}{dæ} = \frac{f_N}{S_N\sqrt{2N}}\exp\left[-\frac{1}{2}\left(\frac{æ - \varepsilon_N}{S_N}\right)\right], \tag{14}$$

where S_N, f_N and ε_N are material constant.

As you can see for use of GTN-model it is necessary to identify seven parameters or six parameters if ε_N is assumed to be equal zero. Moreover in common case f_c depends on stress triaxiality. It is increase number of constants. If the criterion (Eq. 6) is used we need to identify three constant, namely ρ_v^{max}, σ_d and V_{nuc}^{def} (initial volume of deformation void).

Of course, as for both criterion (Eq.6) and GTN-model function $\sigma_S(æ)$ should be known. So it is clear that the use of criterion (Eq. 6) is much simpler than GTN-model.

3. Simulation of material fracture under different conditions of irradiation and testing

The weld metal of 18Cr-10Ni-Ti steel in the initial and irradiated conditions was chosen as an object for the use of the model. Welding was performed with the use of 19Cr-11Ni-3Mo welding wire without subsequent heat treatment. Weld metal specimens were irradiated in the BOR-60 reactor by neutron doses in the range from 6-7 to 46 dpa at a temperature T_{irr}=320-340°C [11].

As the criterion of fracture of a smooth cylindrical specimen the fracture of the central fibre of a specimen neck was taken. To describe the dependences characterizing SST in the central fibre of a specimen neck, $q_m(æ) \equiv \frac{\sigma_m}{\sigma_{eq}}$ and $q_1(æ) \equiv \frac{\sigma_1}{\sigma_{eq}}$ the Bridgman's formulas [12] were used. Over the range of T_{test}=80-495°C the values of fracture strain ε_f^{calc} were calculated on the basis of the condition (Eq. 6). Model parameters are assumed as temperature independent. Fig. 1a shows the experimental data and the dependence $\varepsilon_f^{calc}(T_{test})$. As input data generalized stress-strain curves (SSCs), calculated by equations presented in [11] were used. Values of model parameters are presented in [13, 14].

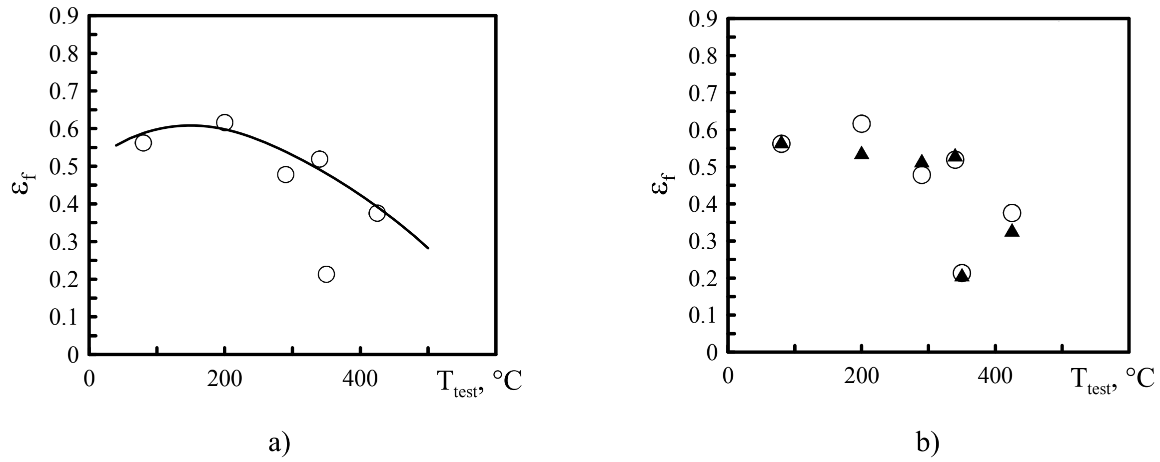

Figure 1. Temperature dependence of the fracture strain of material irradiated by the dose D=46 dpa at T_{irr}=330-340°C: ○ - experimental data, (a) curve - calculated by the model with regard for generalized stress-strain curves [11]; (b) ▲ - points calculated by the model on the basis of individual SSC

Additional calculations ε_f^{calc} were performed for each temperature taking into accounts individual SSCs, obtained from test of each specimen. Results of performed calculations for each test temperature presented on the Fig. 1b. As is seen from Fig. 1, a good agreement between the experimental data and results calculated by the model is observed. The presented data shows that with invariant values of σ_d and ρ_v^{max} the model makes correct predictions of the value ε_f^{exp} at different T_{test} especial with taking into account the peculiarities of individual stress-strain curves for each T_{test}. Thus the effect of T_{test} on ε_f is basically determined by the influence of strain hardening on the realization condition of a plastic collapse of a unit cell.

For analysis of swelling effect and verification of model the weld metal specimens irradiated by a dose of 49 dpa at T_{irr}=400-450°C [15] were used. Swelling of these specimens varies from 3 up to 7%.

Numerical simulation of the influence of vacancy void volume fraction on fracture strain is based on the following propositions:

(1) the SSC for a material matrix, i.e. material without vacancy and deformation voids is invariant to swelling and irradiation temperature and depends only on a neutron dose and test temperature;

(2) when calculating fracture strain for each temperature the individual values of swelling for each specimen [15] were used;

(3) values of the parameters σ_d and ρ_v^{max} are determined from the equality condition $\varepsilon_f^{exp} = \varepsilon_f^{calc}$ at T_{irr}=320-340°C (i.e. without swelling [11, 15]) and T_{test}=80°C, i.e. the same way as described for analyzing of test temperature effect.

The results of the calculation of fracture strain in the absence and existence of swelling are shown in Fig. 2. It is seen from the figure that there is a close coincidence of the experimental and calculated data for specimens without and with swelling (for specimens without swelling comparison of ε_f^{exp} and ε_f^{calc} was shown above in Fig. 1). The obtained results suggest that a decrease of ε_f at T_{irr}=400-450°C compared with ε_f at T_{irr}=320-340°C is connected exclusively with vacancy void volume fraction that determines material radiation swelling. It should be noted that nonmonotonic of the dependence $\varepsilon_f^{exp}(T_{test})$ at T_{irr} =400-450°C is evidently determined by the inhomogeneity of specimens swelling. At the same time the average value of fracture strain $\bar{\varepsilon}_f$ over a temperature range of 80-425°C obtained experimentally approaches the calculated value: $\bar{\varepsilon}_f^{exp}$=0.26, $\bar{\varepsilon}_f^{calc}$=0.25.

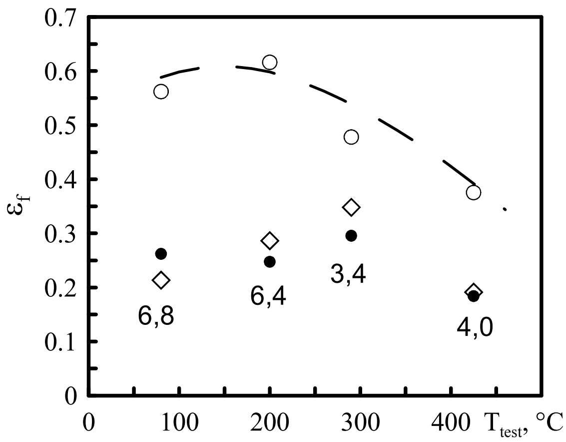

Figure 2. Temperature dependences ε_f^{exp} and ε_f^{calc} for weld metal with and without swelling; the digitals denote swelling of specimens as a percentage: ○ - fracture strain of weld metal without swelling (experiment); ◇ - fracture strain of weld metal with swelling (experiment); ● - calculated value of fracture strain of weld metal with swelling; ——— - calculated temperature dependence of fracture strain of weld metal without swelling.

4. Analysis of an irradiation effect on fracture toughness

To estimate the influence of SST in the dependence $\varepsilon_f(D)$ let us compare the dependence $\frac{\varepsilon_f}{\varepsilon_f^0}(D)$

obtained on the basis of test data processing of smooth cylindrical tensile specimens and the dependence $\frac{\varepsilon_{f\_crack}}{\varepsilon^0_{f\_crack}}(D)$ calculated by the model. For ε_{f_crack} let us take ε_f^{calc} calculated for the stress state typical for a material near a crack tip on the line of its extension. The ε_f^0 and $\varepsilon^0_{f\_crack}$ is fracture strain of material in initial condition with regard to corresponding SST.

Calculation of q_m(æ) and q_1(æ) for tensile specimens was made according to Bridgeman's formulas [12], while calculation for a material near a crack tip was made by the dependences proposed in [16]. The calculation by the model $\frac{\varepsilon_{f\_crack}}{\varepsilon^0_{f\_crack}}(D)$ was made for T_{test}=290°C. The choice of such temperature is connected with the available representative data on $J_c(D)$ for T_{test} = 290-350°C [17]. Table 1 presents the calculation results of $\frac{\varepsilon_f}{\varepsilon_f^0}$ by equation presented in [11] and $\frac{\varepsilon_{f\_crack}}{\varepsilon^0_{f\_crack}}$ calculated by the model.

Table 1. The values $\frac{\varepsilon_f}{\varepsilon_f^0}$, $\frac{\varepsilon_{f\_crack}}{\varepsilon^0_{f\_crack}}$ and $\frac{J_c}{J_c^0}$ at different doses and for the same T_{test}=290°C.

D, dpa	Stress state			σ_{flow}, MPa	$\frac{J_c}{J_c^0}$ (calc)	$\frac{J_c}{J_c^0}$ (exp)
	in the centre of a tensile specimen neck	near the crack tip				
	$\frac{\varepsilon_f}{\varepsilon_f^0}$	ε_{f_crack}	$\frac{\varepsilon_{f\_crack}}{\varepsilon^0_{f\_crack}}$			
0	1	0.0671	1	413	1	1
27	0.480	0.0055	0.082	883	0.175	0.169
46	0.480	0.0056	0.083	883	0.177	0.164

On the basis of above calculations it is possible to estimate a fall of J_c with an increasing dose. Taking into account the approximate dependences $\delta \sim \frac{J}{\sigma_{flow}}$ where δ is a crack opening and $\varepsilon^p \sim \frac{\delta}{r}$ where r is the distance from a crack tip the value J_c under ductile fracture may be presented in the form similar to the proposed in [9]:

$$J_c = \eta \cdot \sigma_{flow} \cdot r_f \cdot \varepsilon_{f\_crack}, \tag{15}$$

where J_c is the critical value of J-integral, r_f is a process zone size, ε_{f_crack} is a fracture strain near the crack tip determined with regard to SST typical for a crack, η is some numerical coefficient, σ_{flow} is the flow strength

$$\sigma_{flow} = \frac{\sigma_Y + \sigma_{ul}}{2}, \tag{16}$$

where σ_Y is yield strength, σ_{ul} is ultimate tensile strength.

Assuming that process zone size r_f is invariant to material condition calculation of a relative decrease of J_c may be determined on the basis of the following expression

$$\frac{J_c}{J_c^0} = \frac{\varepsilon_{f\_crack}}{\varepsilon_{f\_crack}^0} \cdot \frac{\sigma_{flow}}{\sigma_{flow}^0}, \tag{17}$$

where J_c is a critical value of the J-integral for irradiated material, J_c^0 is the critical value of the J-integral for material in the initial condition, σ_{flow} is calculated on the basis of dependencies presented in [11].

The calculation performed by the model at T_{test}=290°C was compared with the experimental data presented in [17] (See Table 1).

As it seen from the presented results, a decrease of ε_f with an increasing dose is considerably enhanced with increasing stress state triaxiality. Thus, for the triaxiality typical for a tensile specimen with D=46 dpa ε_f decreases by half compared to an unirradiated condition, while for the triaxiality typical for material near a crack tip a decrease of ε_f reaches 12 times. In other words, the influence of SST increases with a growth of a neutron dose. Calculation of ε_f with regard to the influence of SST on dependence $\varepsilon_f(D)$ makes possible to describe adequately the change of material fracture toughness under irradiation.

In order to investigate the influence of radiation swelling on J_c we determined the dependences $\varepsilon_{f\_crack}(S_w)$ for different neutron doses from 6 to 46 dpa.

The value of a relative decrease of $\bar{J}_c$ resulted from the value S_w was calculated by the formula

$$\bar{J}_c = \frac{J_c(S_w)}{J_c(S_w = 0)} = \frac{\varepsilon_{f\_crack}(S_w)}{\varepsilon_{f\_crack}(S_w = 0)} \cdot \frac{\sigma_{flow}(S_w)}{\sigma_{flow}(S_w = 0)}, \tag{18}$$

According to [11], $\sigma_{flow}(S_w)$ can be calculated by the formula

$$\sigma_{flow}(S_w) = \sigma_{flow}(S_w = 0) \cdot \left(1 - \left(\frac{S_w}{1 + S_w}\right)^{2/3}\right), \tag{19}$$

Fig. 3 shows the dependence $\bar{J}_c(S_w)$ for different neutron doses. It is seen from the figure that the value $\bar{J}_c$ practically does not depend on a neutron dose, but depends only on the value of swelling S_w.

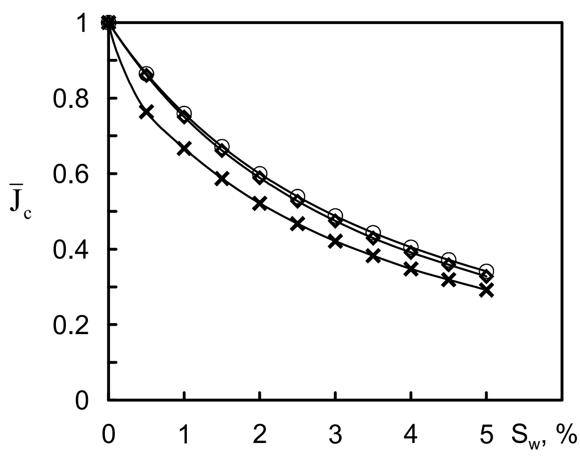

Figure 3. Calculative dependence of relative fracture toughness on radiation swelling for different neutron doses: ○, ———— - D=6 dpa, ◇, — — — - D= 27 dpa, ×, — · — · — - D =46 dpa

At present very few data on swelling effect on fracture toughness are available. That's why prediction by the model needs experimental verification.

5. The swelling effect on ultimate strength of austenitic steel

There are some papers in which the effect of swelling on ultimate strength of irradiated austenitic steels is investigated. According to these papers when swelling reaches some critical value the sharp embrittlement of austenitic steels is observed so that smooth tensile specimens rupture at $\sigma < \sigma_{0.2}$. For example, ultimate strength of irradiated 18Cr-10Ni-Ti steel decreases by 5 times when swelling of steel increases from 17 to 25% [18] (See Fig. 4). It is necessary to note that fracture mode for the considered cases is ductile due to vacancy voids coalescence.

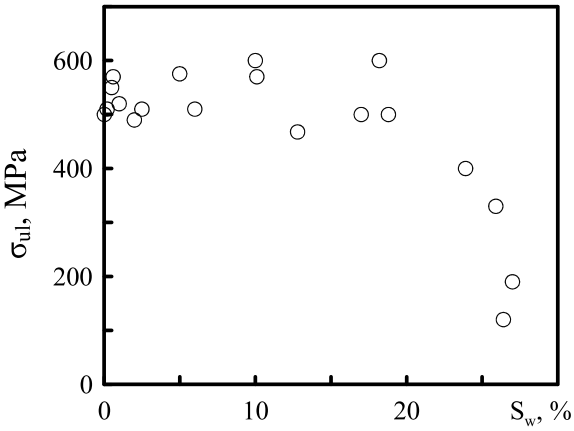

Figure 4. Ultimate strength of irradiated 18Cr-10Ni-Ti steel depending on swelling (T_{test}= 400–500°C) [18]

The widespread explanation of such behavior of material is reduction of specimen net-section due to vacancy voids. But in this case minimal value of ultimate strength of material with swelling σ_{ul} may be calculated by

$$\sigma_{ul} = \left(1 - \overline{A}_v\right) \cdot \sigma_{ul}^m , \tag{20}$$

where $\overline{A}_v = \left(\frac{S_w}{1 + S_w} \right)^{2/3}$ – average area of vacancy voids; σ_{ul}^m – ultimate strength of material without swelling.

Estimation with (Eq. 20) shows that minimum value of σ_{ul} at S_w=30% is equal to 315 MPa. It is clear that this value much higher than experimental values, so the above explanation is insufficient.

According to model proposed by us the embrittlement of a material is caused by two processes. The necessary process is formation of inhomogeneous of vacancy voids distribution that is a result of voids coalescence at some level of swelling. This process may lead to local fracture at low stress, i.e. to microcrack initiation under low stress. Unstable growth of this microcrack up to macro-fracture (fracture of specimen) without increase of stress is considered as sufficient condition for sharp embrittlement. This unstable growth is caused by nano-size of vacation voids and void ligaments when material is loaded in "process zone" Z with very small sizes (~80÷400 nm) being more less than grain size. We have called such mechanism as "running collapse mechanism" (RCM).

According to papers [19, 20] for some value of swelling S_w = $(S_w)_{inh}$ vacation voids begin to coalesce. Void coalescence results in significant inhomogeneity of voids distribution over a material. Voids distribution inhomogeneity is described by the following formula [21]

$$\frac{S_w^{max}}{\tilde{S}_w} = \begin{cases} 1 \quad \text{for} \quad \tilde{S}_w < (S_w)_{inh} \\ \exp\left(\alpha \cdot \left[\tilde{S}_w - (S_w)_{inh}\right]^2\right) \quad \text{for} \quad \tilde{S}_w \geq (S_w)_{inh} \end{cases}. \tag{21}$$

where S_w^{max} is maximal local swelling (in volume of grain); $\tilde{S}_w$ is average swelling of specimen; α is material constant.

In a region with swelling about S_w^{max}, fracture occurs at stress $\sigma_N^{collaps} < \sigma_Y$ and disk-shaped microcrack initiates with size equal to grain size. Fracture stress $\sigma_N^{collaps}$ is calculated by the collapse criterion (See (Eq. 6). This microcrack begins to grow due to ductile fracture of moving "process zone" without increasing stresses. It is possible as the fracture strain of material with vacancy voids is very small and level of local stress and strain in very small "process zone' is sufficiently high.

Figure 5 shows the calculation of ultimate strength of material as a function of radiation swelling.

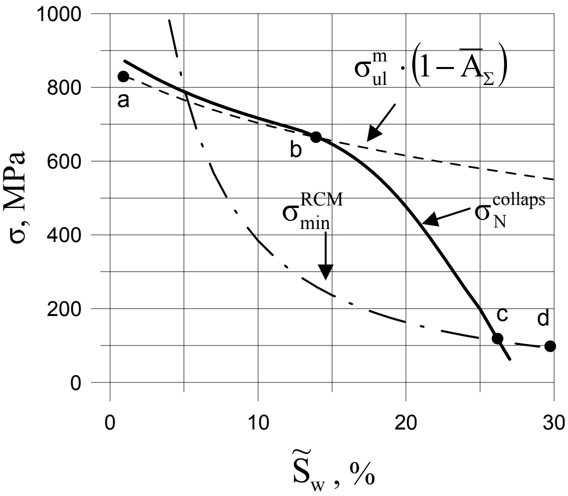

Figure 5. Calculation of ultimate strength of material as a function of swelling $\tilde{S}_w$ (a-b-c-d line):

σ_{ul}^{m} – ultimate strength of material without swelling;

$\sigma_N^{collaps}$ – stress corresponds to fracture of grain with swelling S_w^{max} (disk-shaped crack nucletion);

σ_{min}^{RCM} - minimal stress for running collapse mechanism;

$\sigma_{ul}^{m} \cdot \left(1-\overline{A}_\Sigma\right)$ – ultimate strength decrease due to net-section decrease.

6. Conclusions

(1) The model of ductile fracture was developed, which makes it possible to describe the influence of stress state triaxiality, neutron irradiation and radiation swelling on the critical parameters controlling fracture: fracture strain ε_f and the critical value of J-integral J_c.

(2) Predictions were made on the influence of a neutron dose on ε_f and fracture toughness J_c. It was shown that as stress state triaxiality increases the irradiation influence on ε_f increases. The calculation results of J_c showed that this parameter for D ≥6 dpa decreases by ~6 times.

This prediction is in complete agreement with the experimental data.

(3) The model predicts a severe decrease of J_c with a growth of swelling in relation to J_c of a material irradiated under the condition when radiation swelling is absent.

(4) It is shown that the root causes of ductile fracture of highly irradiated austenitic steels at low stresses (less than yield strength) and sharp reduction of ultimate strength are the following:
- formation of inhomogeneous distribution of vacancy voids at some critical level of swelling $(S_w)_{inh}$;
- fracture in "process zone" which has nano sizes (80-400 nm) considerably less than grain size.

(5) Initiation of fracture in a grain with high level of swelling and unstable microcrack propagation result in fracture of specimen at stress less than yield strength. Unstable microcrack propagation occurs due to local ductile fracture of moving "process zone" (this mechanism is named as "running collapse mechanism").

(6) The proposed model allows one to predict the swelling effect on sharp reduction of ultimate strength.

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