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# Master curve in upper region of ductile brittle transition: a modification based on local damage approach

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## Abstract

The fracture behaviour of ferritic/ferritic martensitic steels in Ductile to Brittle Transition (DBT) region is well captured by Master Curve approach, except in the upper region of transition due to ductile tearing prior to cleavage. The fracture toughness behavior in the upper region of DBT is generally censored by Master Curve. In this work the Master Curve approach is modified to extend its applicability to the upper region of transition. The ductile tearing in the upper region of transition, increased sampled volume and constraint increment are addressed in this work using constraint parameter  $T_{stress}$  and numerical analyses using GTN damage.

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Keywords: Master Curve; Local damage; ductile brittle transition; VUMAT; ABAQUS

## 1. Introduction

The Master Curve (MC) approach models cleavage and assumes self-similarity of stress field at the crack front. This single fracture parameter, KJC, based approach restricts its applicability to lower region of transition where insignificant amount of ductile tearing precedes cleavage. In upper region of transition, the increasing active volume comprises a part of volume ahead of crack tip, changing to plastic wake after ductile tearing and other which contributes to cleavage. The increment in constraint with associated change in ligament length with Ductile Crack Growth (DCG) increases the number of potentially critical carbides for cleavage succeeding eventually in cleavage fracture.

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Nomenclature					
в	dimensionless constants in DCG modified cleavage failure probability by Wallin				
u u	mean of distribution of voids nucleation				
v	Poisson's ratio				
$\sigma_{flow}$	average of yield strength and ultimate tensile strength				
$\sigma_{YS}$	Yield strength				
$\sigma_{std}$	standard deviation of distribution of void nucleation sites				
а	crack length				
$\Delta a$	ductile crack growth prior to cleavage in ductile to brittle transition region				
fc	critical value of void volume fraction to incorporate void coalescence				
nT	thickness of specimen in terms of n inch				
q1, q2	constant in GTN theory used to define yield function				
Α	athermal toughness contribution in 100 MPa.m1/2 toughness at reference transition temperature				
В	thickness of fracture specimen				
С	empirical constant in exponential variation of thermal part of 100 MPa.m <sup>1/2</sup> toughness at reference				
	transition temperature				
Е, Е'	elastic modulus for plane stress and plane strain respectively				
$K_0$	fracture toughness at 63.2% cleavage probability				
$K_{JC}$	elastic plastic fracture toughness based on J-integral				
K <sub>min</sub>	threshold fracture toughness below which cleavage cannot occur				
K <sub>JC,med</sub>	median of elastic plastic fracture toughness data generated in transition region				
$K_{JC,nT}$	elastic plastic fracture toughness based on J-integral for specimen of thickness (n) inch				
K <sub>JC,lim</sub>	limit of fracture toughness defined in ASTM E1921-13a				
$\mathbf{K}_{JC,\Delta a}$	fracture toughness of a specimen for which stable crack growth is higher than 0.05 times of ligament or 1				
ת	mm (whichever is smaller)				
$P_f$	Probability of cleavage failure				
	Second terms of William's stress function				
1 stress	Change in Tatrage as a function of increasing arealy length				
$\Delta I$ stress $W$	Width of a fracture specimen defined in ASTM E1820				
W.	Constant in DCG modified cleavage failure probability				
	Ductile to brittle transition				
MC	Master Curve				
	Illtimate tensile strength				
VS	Vield strength				
GTN	Gurson Tvergaard and Needleman				
CT	Compact tension				
TPB	Three point bend				
DCG	Ductile crack growth				
FEA	Finite element analysis				

In the conventional MC approach the fracture data associated either with constraint loss or DCG prior to cleavage are censored with the limiting values described in ASTM E1921-13a. The censoring increases the number of tests required for determination of reference transition temperature. Moreover, the true fracture behaviour of upper region of transition is not captured by conventional Master Curve approach. The censoring of dataset belonging to cleavage fracture with prior DCG instead of capturing the real fracture behaviour, underestimates the material potential. The general expression of fracture toughness with temperature given by Master Curve is as in Eq. (1).

$$K_{JC,1T} = A + (A_0 - A) \cdot \exp[C \cdot (T - T_0)]$$
<sup>(1)</sup>

where  $K_{JC}$  is the elastic plastic fracture toughness size adjusted to a specimen of 1 inch (1*T*) thickness.  $A_0$  and  $T_0$  are the reference values of fracture toughness and temperature respectively. Empirical constant of exponential function is *C*, whereas *A* is the fitting parameter of Master Curve and *T* represents test temperature. In general convention of Master Curve methodology,  $A_0$  is 100 MPa m<sup>1/2</sup>, *C* is 0.019 °*C*<sup>1</sup> and *A* is 30 MPa m<sup>1/2</sup>. The probability of cleavage failure defined in Master Curve method is shown in Eq. (2).

$$P_{f} = 1 - \exp\left[-\frac{B_{xT}}{B_{1T}} \left(\frac{K_{JC} - K_{\min}}{K_{0} - K_{\min}}\right)^{4}\right]$$
(2)

The fracture tests for determination of reference transition temperature  $T_0$  are carried out in the estimated range of -50 °C $\leq T$ - $T_0\leq 50$  °C. The dataset is checked for validity using the criteria shown in Eq. (3a) and Eq. (3b).

$$K_{JC} \ge K_{JC, \lim} = \sqrt{\frac{E \cdot b_0 \cdot \sigma_{YS}}{M \cdot (1 - \nu^2)}}$$
(3a)

$$\Delta a \le \frac{0.05 \cdot b_0}{1mm} \tag{3b}$$

The invalid dataset is censored with  $K_{JC,lim}$  value and  $K_{JIC}$  or maximum valid  $K_{JC}$  for the respective validity criteria. The dataset after censoring is analysed for determination of  $T_0$  using maximum likelihood estimation method. Further details of the MC analysis can be found in the work of Wallin (1999).

#### 1.1. Master Curve in upper region of ductile to brittle transition

In the upper region of transition the ductile tearing occurs due to the well-known mechanism of void nucleation, growth and coalescences which is a result of large strain plastic deformation at the crack tip. This type of cleavage accompanied by prior DCG can occur in the range of MC applicability, if the constraint loss is more. The constraint in the process of ductile tearing increases due to decreasing ligament length and also criticality of the inhomogeneities such as carbides which causes cleavage later.

To include the fracture behavior of materials in upper region of transition, Wallin (1989) has suggested a modification which works for prior DCG of very small amount. The change in failure probability in context to Master Curve approach is also studied by Tagawa et al. (2010), revealing a change in slope of scatter bounds. The analytical contribution of sampled volume in case of prior DCG is studied by Brückner and Munz (1984). The study of Brückner and Munz (1984) and Wallin (1989) on the probability of cleavage failure shows similar expressions of cleavage failure probability in presence of prior DCG as in Eq. (4a) and Eq. (4b).

Wallin's expression (Eq. (4b)) assumes that the effective active volume grows with increased loading, whereas Brückner and Munz's expression (Eq. (14a)) assumes the active volume to be constant after DCG start. Wallin found that the probability of failure in case of very small prior DCG can be taken care of by a modified probability distribution as shown in Eq.(5).

$$\ln(\frac{1}{1-P_f}) = (\frac{K_{JC(i)}}{K_0})^4 + \frac{1}{K_0^4 \cdot W_1} \cdot \int_0^{\Delta a} f(\Delta a)^2 \cdot \partial(\Delta a)$$
(4a)

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$$\ln(\frac{1}{1-P_f}) = (\frac{f(\Delta a)}{K_0})^4 + \frac{2 \cdot \sigma_{flow}^2}{K_0^4 \cdot \beta} \cdot \int_0^{\Delta a} f(\Delta a)^4 \cdot \partial(\Delta a)$$
(4b)

$$\ln(\frac{1}{1-P_f})^{1/4} = (\frac{K_{JC(i)}}{K_0})(1 + \frac{2 \cdot \Delta a \cdot \sigma_{flow}^2}{K_{JC(i)}^4 \cdot \beta})^{1/4}$$
(5)

where  $\Delta a$  is the amount of DCG prior to cleavage,  $\beta$  is a fitting parameter,  $W_1 = K_{JC}^2 \cdot \beta$ , and  $\sigma_{\text{flow}}$  is the flow stress calculated as average of Yield strength (YS) and Ultimate Tensile Strength (UTS) and  $f(\Delta a)$  is a function dependent on DCG affecting the active volume responsible for cleavage ahead of crack tip.

## 1.2. Modification of Master Curve in upper region of ductile to brittle transition

The fracture behavior of ferritic steels in upper region of transition i.e. the region where cleavage occurs with prior DCG is re-investigated by using the biggest dataset in transition region of reactor pressure vessel steel known as Euro fracture dataset credited to Heerens and Hellman (1999), Chaouadi (1998) and Heerens and Hellman (2002). The energy balance for cleavage with prior DCG can be written as in Eq. (6).

$$\frac{K_{JC,\Delta a=x}^2}{E'} = \frac{K_{JC,\Delta a=0}^2}{E'} + \frac{1}{\Delta a} \int_{\Delta a=0}^{\Delta a=x} \frac{K_{JC}(\Delta a)^2}{E'} \cdot d(\Delta a)$$
(6)

To have the value of second term in Eq. (6), the Euro fracture dataset is re-investigated as shown in Fig. 1. The effect of temperature in transition region and the effect of size is shown in Fig. 1(a) and 1(b) respectively.



Fig. 1. (a) $K_{JC}$  vs.  $\Delta a$  for 0.5T-CT in range of -40 to 0<sup>o</sup>C and (b) for 0.5T, 1T and 2T CT specimens at -40<sup>o</sup>C.

It is evident from Fig. 1 that in range of  $0.40^{\circ}$ C for 0.5T-CT specimens the variation of  $K_{JC}$  with  $\Delta a$  shows a single curve and can be described as a function of  $\Delta a$  alone. However, the thickness of the specimen alters the behaviour as shown in Fig. 1(b). The region may be attributed to change in constraint and probability of finding inhomogeneities for differently sized specimens. Observation can also be made from Fig.1 (a) and 1(b) that the  $\Delta a$  increased when tests were carried out in upper region of transition. The similar increment was shown for smaller specimens. The behaviour independent of temperature can be explained by change in constraint associated with  $\Delta a$ .

The material under loss of constraint, which may occur at higher temperatures or smaller thickness, on loading causes blunting of crack tip followed by cleavage if the amount of work hardening during blunting activates the critical carbides for cleavage. If this situation is not achieved, blunting is followed by ductile tearing. This ductile tearing also increases the constraint as the a/W increases. Finally, after required amount of  $\Delta a$  the carbides become critical and results in cleavage.

In order to include the failure probability of cleavage with significant amount of prior DCG, a constraint parameter  $\Delta T_{\text{stress}}$  (the change in  $T_{\text{stress}}$  is only due to change in ligament length while ductile tearing) based function is used as a trial function to modify the probability of cleavage failure in upper region of transition. The  $T_{\text{stress}}$  based trial function is shown in Eq. (7) and the modified cleavage failure probability is shown in Eq. (8).

$$f(\Delta T_{stress}) = (1 + \begin{vmatrix} T_{stress} \\ \sigma_{YS} \end{vmatrix})$$
(7)

$$P_{f} = 1 - \exp\left[-\frac{B_{xT}}{B_{1T}} \cdot \left(1 + \left|\frac{T_{stress}}{\sigma_{YS}}\right|\right) \cdot \left(\frac{K_{JC} - K_{\min}}{K_{0} - K_{\min}}\right)^{4}\right]$$
(8)

The modified cleavage failure probability of Eq. (7) is investigated on experimental results of newly developed Indian Reduced Activation Ferritic/Martensitic Steels (In-RAFMS). The same has also been investigated on Euro Fracture dataset and the numerical results obtained by modelling Three Point Bend (TPB) fracture specimen.

#### 2. Numerical analysis

The numerical analysis to simulate prior ductile crack growth to cleavage, was carried out using a ductile damage. The failure criterion was ductile damage dependent. The load displacement response of the model was used to calculate  $K_{JC}$  by assuming cleavage to occur at each increment point. The numerical simulation is carried out for specimens loaded in bending, however as in Eq. (7) unsigned value of  $\Delta T_{stress}$  is used, the function behaviour becomes independent of type of loading, although the amount of change of f ( $\Delta T_{stress}$ ) would be different for loading in tension and in bending.

In this work, to introduce the ductile crack growth prior to cleavage, a user material program VUMAT which can be coupled with ABAQUS FEA software credited to Hibbit et al. (2007) was written. The VUMAT subroutine calculated the yield function and void volume fraction in each elements locally using GTN theory based on the work of Gurson (1977), Tvergaard (1981) and Tvergaard and Needleman (1984). The element deletion option was used with VUMAT to induce ductile crack growth.

The calibration of GTN parameters were carried using the initial values from the work of Stratil et al. (2014) on Eurofer97. The calibrated values of GTN parameters for the In-RAFMS corresponding to -110 °C tensile property is shown in Table. 1. The geometry modeled with boundary conditions and mesh is shown in Fig. 2(a). The final crack growth can be visualized in Fig. 2(b).

Fracture model	GTN Parameters						
VUMAT	q1	q2	$\mathbf{f}_{\mathbf{f}}$	fc	μ	$\sigma_{\text{std}}$	$f_0$
	1.06	0.931	0.08	0.01	0.3	0.1	0.00088

Table 1. GTN parameters used in subroutine VUMAT for TPB geometry

The TPB specimen geometry modelled was  $5 \times 10 \times 20$  mm<sup>3</sup>. The tensile property corresponding to 4mm diameter round bar tensile specimen of In-RAFMS with gauge length of 20 mm tested at -110°C was used as input in the form of true stress and plastic strain with incremental plasticity. The mesh was refined in the near crack region and only this region was assigned VUMAT property. The VUMAT subroutine was tested to reciprocate tensile behavior

and was compared for void volume fraction with in-built GTN algorithm of ABAQUS package. The model was solved using 20 noded brick elements with full newton algorithm of non-linear solution.



Fig. 2. (a) TPB geometry modeled in ABAQUS using VUMAT subroutine; (b) simulated ductile crack growth of 2.79mm.

#### 3. Material and Experimental details

The In-RAFMS is a ferritic/martensitic steel in the category of fusion reactor first wall material, such as Eurofer97, F82H-mod. The chemical composition of In-RAFMS is shown in Table 2. The specimens were fabricated from 12mm sheet which was solutionized at 1250K for 30 minutes and tempered after air cooling to 1033K for 60 minutes.

Table 2. Chemical composition of In-RAFMS										
С	Cr	W	V	Та	Si	Mn	S	Ν	Ni,Sn,Co	
0.08	9.15	1.37	0.24	0.08	0.026	0.53	0.002	0.02	≤0.004	

The experimental studies were performed on 0.5T-CT and 0.2T-TPB specimens of In-RAFMS. The fracture tests were carried out in a closed environmental chamber connected with universal testing machine at strain rate of  $4.16 \times 10^{-4}$ s<sup>-1</sup>. The fracture tests for CT specimens were performed at -50°, -60°, -70°, -80°, -100 °C and -120 °C. The test for TPB specimens were carried out at -110 °C, -120 °C, -130 °C and -140 °C. As the TPB specimens were of smaller thickness (0.2T), the testing temperature was chosen to be lower than that for CT specimens.The temperature was maintained with ±3 °C accuracy by recirculating liquid N<sub>2</sub> in the environmental chamber fixed with the universal testing machine.

## 4. Results and Discussion

The numerical analysis of TPB specimen had a final crack growth of 2.79 mm measured from user interface using 9 point average method. At each increment the DCG was measured and the  $K_{JC}$  was calculated using load-load line displacement response. Each value corresponding to each increment was assumed to be an event of cleavage failure after corresponding DCG. The events were assigned ranks and rank probability was calculated. The behavior of rank probability against  $K_{JC}$  and functions of  $K_{JC}$  and  $\Delta a$  of Wallin's DCG correction from Eq. (5) and modification investigated in this work using Eq. (8). The behavior is shown in Fig. 3.



Fig. 3. Conventional MC and Mod-MC plot of (a) 0.5T CT (b) 1T CT (c) 2T CT specimens



Fig. 4. (a) MC and Mod-MC of In-RAFMS 0.5T CT specimens and (b) TPB specimens.

It is evident from Fig. 3(a) that the behavior of  $K_{JC}$  with  $\ln[1/1-P_J]^{1/4}$  becomes non-linear at higher amount of  $\Delta a$ . The correction of Wallin as shown in Eq. (5) shows greater range of linearity than conventional MC variation. The modified probability of cleavage failure expressed by Eq. (7) shows full range of linear behavior and a coupling of trial function with Wallin's correction shows a decreasing slope as expected due to repetition of correction for DCG. The initial region of non-linearity is attributed to initiation toughness and blunting. From Fig. 3(a), therefore, it is clear that the trial function in form of Eq. (8) can be used for significant amount of DCG. The modified MC (Mod-MC) is applied on the Euro fracture dataset in the category of thickness of the specimens. The MC and Mod-MC plots for 0.5T, 1Tand 2T specimens are shown in Fig. 3(b), 3(c) and 3(d). The modified as well as conventional MC analysis was conducted on In-RAFMS TPB and CT specimens. The MC plot is shown in Fig. 4.

For CT specimens the conventional MC resulted in  $T_0$  of -123 °C, however, Mod-MC resulted in  $T_0$  of -120 °C. The two results had no significant difference, however, in case of TPB specimen; the  $T_0$  obtained by conventional MC was -123 °C. This value is significantly higher than that obtained by Mod-MC, which is -148 °C. This is attributed to the number of censored data in case of TPB and CT specimens. In case of CT specimens out of 26, 12 were invalid in conventional MC analysis, whereas in case of TPB 13 were invalid out of 53 tests. In Mod-MC analysis the partial censoring made any data which had significant amount of crack growth valid with  $T_{stress}$  correction. Another reason for this difference in case of TPB is due to the role of  $T_{stress}$  which is positive unlike in case of CT specimens.

### 5. Conclusions

Master Curve methodology is modified with a constraint based function of  $T_{stress}$  for its application in upper region of DBT. The modification is justified using numerical analysis and is applied to Euro Fracture dataset as well as fracture data generated on TPB and CT specimens of In-RAFMS. The Mod-MC shows potential of estimating  $T_0$ close to that obtained by conventional MC with increased validity window. In case of TPB geometry on the dataset of In-RAFMS, Mod-MC results in a lower  $T_0$ , which is attributed to the positive nature of  $T_{stress}$ , the size difference of TPB with CT and the number of invalid data in each dataset.

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