ESTIMATION OF EFFECTS OF SPECIMEN GEOMETRY AND SIZE ON THE DUCTILE-TO-BRITTLE TRANSITION TEMPERATURE USING COMBINED NONLOCAL DUCTILE DAMAGE AND CLEAVAGE FRACTURE MODELS

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ABSTRACT

The pressure vessel and piping components may be subjected to operation in the ductile-to-brittle transition regime of the material due to increase in the transition temperature. This increase can be due to irradiation embrittlement, various other material aging and degradation mechanisms taking place in a nuclear reactor environment. The two mechanisms that compete with each other in the failure process are: ductile and cleavage fracture. From fracture mechanics point of view, fracture toughness of the material must be adequate to prevent the failure. However, there is considerable scatter observed in the fracture toughness data and the analyst must account for this in the safety analysis. Master curve approach according to ASTM E1921 standard is popularly employed for this purpose. However, it requires the data for transition temperature T₀, which is dependent upon the specimen geometry and loading configurations employed in the laboratory tests. Its transferability to safety analysis of components is questionable.

In this work, the nonlocal Rousselier’s damage model along with Beremin’s model has been used to simulate the fracture toughness variation in the DBTT region for two different types of nuclear pressure vessels steels. In addition, the effects of specimen type, size, crack depth and loading conditions on the fracture toughness variation in the DBTT region have been evaluated. Extensive experiments have been conducted on these different materials and specimens. The experimental data have been compared with the results of numerical simulation. It is demonstrated that the scatter and fracture toughness variation can be predicted once we know the material stress-strain data at different temperatures and a single set of Weibull statistics parameters for cleavage of the material. One doesn’t need to evaluate T₀ as a function of specimen geometry, size and loading conditions etc., which is required in case of master curve approach. The model inherently captures the effect of above parameters on the fracture toughness transition curve.

Keywords: Fracture toughness master curve; Ductile-to-brittle transition; Nonlocal formulation

INTRODUCTION

Most of the safety critical components, such as the pressure vessels of nuclear reactors, are made of ferritic grade low-alloy steels. It is widely known that these materials undergo a ductile-to-brittle transition (DBTT) when the temperature is lowered. The DBTT temperature is very low (of the order -60 to -70 deg. C) for the new and un-irradiated materials. However, due to irradiation embrittlement and other material aging and degradation mechanisms, the transition temperature can increase significantly. In the case of an accident scenario such as a loss-of-coolant accident, the unstable propagation of cleavage cracks cannot be ruled out.

The two mechanisms that compete with each other in the failure process in the DBTT regime are: ductile and cleavage fracture. From fracture mechanics point of view, fracture toughness of the material must be adequate to prevent the failure. However, there is considerable scatter observed in the fracture toughness data and the analyst must account for this in the safety calculations.

Master curve approach according to ASTM E1921 standard [1] is popularly employed for this purpose. However, it requires the data for transition temperature T₀, which is dependent upon the specimen geometry and loading configurations employed in the laboratory tests. Its transferability to safety analysis of components is questionable. In view of this, a numerical model which can incorporate the statistical aspects of the combined mechanism of ductile [2] and cleavage fracture in needed. Beremin’s model [3] along with elastic-plastic finite element (FE) analysis is popularly used by the researchers to predict the cleavage fracture probabilities. However, the temperature dependency of the Weibull distribution [4] parameters is an issue.

In this work, Beremin’s model has been combined with nonlocal damage mechanics models [5-7] instead of J2-type elastic-plastic models. When simulating the crack tip stress field at lower temperatures (when stress gradients are large), one needs to use a very fine mesh, which cannot be used in the local damage mechanics models (as the mesh size is pre-defined for a material, which is typically of the order of 0.2mm and is
usually too coarse to correctly capture the low temperature crack tip stress field). Many authors have suggested an empirical variation of Weibull parameters with temperature and used the same for prediction of the transition curve along with elastic-plastic analysis for calculation of Weibull stress. However, the problem lies in the inability to model small amounts of ductile crack growth (before start of unstable cleavage fracture) in the FE analysis. Again, the minimum amount of stable crack growth that can be simulated is of the order of one element size.

In our experiments, we observed that the average stable crack growth (before instability) is of the order of 0.2 mm at -20 deg. C and hence to simulate very small amounts of crack growth (of the order of one-tenth of 0.2 mm), we require mesh sizes of the order of 0.02 mm, for which local damage models cannot be employed. Fracture experiments have been conducted on two different types of nuclear pressure vessel steels using standard specimens. In addition, the effects of specimen type, size, crack depth and loading conditions on the fracture toughness variation in the DBTT region have been evaluated. The experimental data have been compared with the results of numerical simulation.

It is demonstrated that the scatter and fracture toughness variation can be predicted once we know the material stress-strain data at different temperatures and a single set of Weibull statistics parameters for cleavage of the material. One doesn’t need to evaluate $T_0$ as a function of specimen geometry, size and loading conditions etc., which is required in case of master curve approach [8-10]. The model inherently captures the effect of above parameters on the fracture toughness transition curve.

**MESH-INDEPENDENT NONLOCAL MODEL FOR DUCTILE FRACTURE**

In the earlier works, the authors have developed a nonlocal formulation of Rousselier’s model using nonlocal damage $d$ as a nodal degree of freedom in the FE mesh [5-6]. The increment of the nonlocal damage variable $d$ in a material point $\bar{x}$ is mathematically defined as a weighted average of the increment of the local void volume fraction $\dot{f}$ in a domain $\Omega$, i.e.,

$$
\dot{d}(\bar{x}) = \frac{1}{\Psi(\bar{x})} \int_{\Omega} \Psi(\bar{y};\bar{x}) \dot{f}(\bar{y}) d\Omega(\bar{y})
$$

(1)

where $\bar{y}$ is the position vector of the infinitesimally small volume $d\Omega$ and $\Psi(\bar{y};\bar{x})$ is the Gaussian weight function given by

$$
\Psi(\bar{y};\bar{x}) = \frac{1}{8\pi^{3/4}l^3} \exp \left( -\frac{|\bar{x} - \bar{y}|^2}{4l^2} \right)
$$

(2)

The length parameter $l$ in Eq. (2) determines the size of the volume, which effectively contributes to the nonlocal quantity and is related to the scale of the microstructure. The above integral nonlocal kernel holds the property that the local continuum is retrieved if $l \rightarrow 0$. By expanding $\dot{f}(\bar{y})$ in Taylor’s series and substituting in Eq. (1) and doing some algebra, one can obtain the damage diffusion equation as

$$
\dot{d} - f - C_{\text{length}} \nabla^2 d = 0
$$

(3)

where $C_{\text{length}}$ is the characteristic length parameter of the material [43, 44]. The yield function of the Rousselier’s model [30] is modified by substituting the nonlocal damage $d$ in place of the local ductile void volume fraction $f$ as [5]

$$
\phi = \frac{q}{1-d} + D\sigma_d d \exp \left( -\frac{p}{(1-d)\sigma_q} \right) - R\left(\varepsilon_{eq}\right) = 0
$$

(4)

where $D$ and $\sigma_q$ are the parameters of the Rousselier’s model and are constants for a material.

With loading, the void volume fraction evolves from the initial void volume fraction $f_0$ (volume fraction of eligible second phase particles responsible for nucleation of voids upon plastic deformation) in the material. At a critical void volume fraction $f_c$, the voids coalesce with each other and at the final void volume fraction $f_f$, the material points loses its stress carrying capability. Hence, the above three void parameters (i.e., $f_0, f_c$ and $f_f$) are also the material properties of the damage model.

For solving the boundary value problem of the nonlocal damage continuum, one needs to solve the partial differential equation (3) along with the mechanical equilibrium equation. A FE formulation of the above process has been implemented in an in-house code and it has been used for analysis of different types of specimens in this work.
BEREMIN’S MODEL FOR CLEAVAGE FRACTURE

Beremin’s model for cleavage fracture is based on the weakest link concept where the probability of fracture can be represented in general as

\[ P_f = 1 - \exp \left\{ - \int g\left(\frac{\sigma_i}{\sigma_{\text{ref}}}\right) \frac{dV}{V_{\text{ref}}} \right\} \]  

(5)

where \( V \) is the volume of the plastically deformed zone (an essential condition for slip induced nucleation of cleavage micro-cracks) in the component, \( V_{\text{ref}} \) is the reference volume which is taken many times as 0.001 mm³. The function \( g\left(\frac{\sigma_i}{\sigma_{\text{ref}}}\right) \) expresses the probability of failure of an infinitesimal volume \( i \) (having volume \( dV \)) according to the expression

\[ dp_f = g\left(\frac{\sigma_i}{\sigma_{\text{ref}}}\right) \frac{dV}{\ref} \]  

(6)

where \( \sigma_i \) is the maximum principal stress acting at a material point \( i \) in the plastically deformed region having volume \( dV \). According to Beremin’s model [3] (which uses Weibull’s statistics for distribution of defects responsible for triggering cleavage according to Griffith’s theory), the form of \( g\left(\frac{\sigma_i}{\sigma_{\text{ref}}}\right) \) is defined as

\[ g\left(\frac{\sigma_i}{\sigma_{\text{ref}}}\right) = \left(\frac{\sigma_i}{\sigma_u}\right)^m \]  

(7)

where \( m \) and \( \sigma_u \) are the Weibull’s shape and size parameters respectively. Using Eq. (7) in Eq. (5), one can obtain the probability of cleavage fracture \( P_f \) at any given loading as [3]

\[ P_f = 1 - \exp \left\{ - \left(\frac{\sigma_u}{\sigma_{\text{ref}}}\right)^m \right\} \]  

(8)

where the loading parameter is defined as the Weibull stress \( \sigma_u \) and is expressed as [3]

\[ \sigma_u = \left(\sum_{i=1}^{\infty} \left(\frac{\sigma_i}{\sigma_u}\right)^m \frac{V_i}{V_0}\right) \]  

(9)

In the present work, Eq. (8) is used to calculate the probability of cleavage fracture of the CT specimen at different loading levels and at different temperatures, where the Weibull stress will be calculated using the stress field ahead of the growing crack using Eq. (9). The nonlocal Rousselier’s damage model has been used to calculate the crack-tip stress field. The effect of evolution of damage (ductile void volume fraction) on the stress field is taken care of by this model and hence, the effect of prior stable crack growth before initiation of cleavage fracture is modeled implicitly through this framework.

RESULTS AND DISCUSSION

In the DBTT regime, the crack-tip experiences a large stress gradient and hence, the ductile crack growth (of the order of few microns) before unstable cleavage fracture cannot be predicted by the local damage models. This is because of the mesh-dependent nature of the results obtained with these models. In order to use fine mesh in the crack-tip and at the same time, to use ductile damage models, the nonlocal formulation of the Rousselier’s damage model has been used in this work.

![Stress-strain curve at various temperatures](image)

Fig. 1: Stress-strain curve at various temperatures obtained from tensile tests for DIN 22NiMoCr3-7 steel
The results of this model have been demonstrated to be mesh-independent in the earlier works of the authors. Hence, this model along with the Beremin’s model for cleavage fracture has been used to simulate the fracture transition curve for two different types of materials.

**Prediction of fracture transition curve for the pressure vessel steel material-I**

The true stress-strain curve of the material at different temperatures as used in FE analysis is shown in Fig. 1. Other material properties including the Rousselier’s constants, characteristic length parameter and the void volume fractions (initial, final and at coalescence) are shown in Table-1.

Table-1: Material properties of DIN 22NiMoCr3-7 pressure vessel steel

<table>
<thead>
<tr>
<th>Model parameters</th>
<th>Rousselier’s constants</th>
<th>Void parameters</th>
<th>Char. length parameter</th>
<th>E (Young’s mod. in GPa)</th>
<th>V (Poisson’s ratio)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$D$</td>
<td>$\sigma_k$ (MPa)</td>
<td>Initial void volume fraction $f_0$</td>
<td>Void volume fraction at coalescence $f_c$</td>
<td>Final void volume fraction $f_f$</td>
</tr>
<tr>
<td>Value</td>
<td></td>
<td>2</td>
<td>445</td>
<td>0.0003</td>
<td>0.05</td>
</tr>
</tbody>
</table>

Fig. 2: Geometry, dimension and loading conditions for the CT specimen

Experiments have been conducted on standard 1T CT specimens [Fig. 2] at various temperatures in the DBTT regime of the material. The experimental data of fracture toughness $K_{JC}$ has been plotted at various temperatures in Fig. 3. It can be observed that there is a substantial scatter in the fracture toughness data. The scatter is lowest in the lower shelf temperature at -100 deg. C and it increases with temperature. The scatter near the upper shelf region is highest. This is because of the presence of two different processes (i.e., cleavage and ductile fracture) towards the upper-shelf temperature region in the BDTT regime. Each of the fracture processes have inherent scatter. The scatter in initiation of cleavage fracture is due to the scatter in size and distribution of second phase

particles which are responsible for triggering of the same (mainly carbides in these ferritic steels). In case of ductile fracture, the size, distribution and interfacial strength of the inclusions (MnS type) and other second phase particles control the scatter in fracture toughness. As both these processes operate near the right end of the DBTT regime, the scatter is larger compared to pure cleavage fracture in the lower-shelf region. Fig. 3 shows the predicted fracture toughness variation (with temperature) for the 1T CT specimen by two different types of models, i.e. (a) elastic-plastic analysis; and (b) nonlocal damage models.

![Fig. 4: Geometry, dimensions and loading conditions for SEB specimen](image)

For both the methods, FE analysis has been carried out using 3D iso-parametric 20-noded brick elements. The mesh size near the crack-tip has been of the order of 0.02 mm. The Weibull parameters \(m\) and \(\sigma_0\) used in the analysis are 34.6 and 2005 MPa respectively. It can be observed that the scatter evaluated using Weibull stress values computed according to elastic-plastic models are able to predict the observed experimental scatter satisfactorily at the lower-shelf temperature region of -100 to -60 deg. C. However, the predicted scatter is away from the experimental scatter for the temperature beyond this region. This is because of the effect of ductile crack growth (i.e., softening) is not considered in the crack-tip stress fields.

![Fig. 5: Predicted fracture toughness scatter and its variation with temperature for the 1T SEB specimen](image)

The crack-tip stress field as computed by the nonlocal damage model has considered the effect of the ductile crack growth and hence, the predicted fracture toughness scatter compares very with that of experimental data.
The master curve for fracture probability of 5% and 95% has also been plotted along with the experimental and FE results in Fig. 3. It can be observed that the combined nonlocal ductile and cleavage fracture model has been able to predict the experimental data of fracture toughness as well as the master curve very accurately. However, the master curve requires the evaluation of the transition temperature $T_0$ from experimental data and hence, this $T_0$ may be not applicable when the fracture toughness variation of different types of specimens and components are to be predicted. It will be shown in the following sections that the numerical model as discussed in this work is able to predict the effect of specimen geometry, size, crack depth, loading types etc. on the shape of the fracture toughness transition in the DBTT region of ferritic pressure vessel steels.

**Effect of specimen geometry and loading type on the fracture toughness transition curve**

Another specimen type (i.e., a standard single-edged cracked specimen loaded in three-point bending, SEB, as shown in Fig. 4) is considered here for the analysis. The results of the nonlocal model are shown in Fig. 5. The results of analysis are plotted along with the experimental data and master curves. The same set of Weibull parameters as used previously has been used here. It can be observed that the model has been able to predict the experimental scatter satisfactorily. The master curve also compares very well with the predictions of the model.

The fracture toughness transition curves as predicted by the model for both the 1T CT and 1T SEB specimens are also plotted together in Fig. 6. It can be observed that the 50% and 95% failure probability curves differ slightly among the two types of specimens. The two types of specimens see different crack-tip loading conditions and hence, the scatter in fracture toughness curves is slightly different. The scatter is more for the SEB specimen especially in the right hand side of the DBTT regime. This indicates that the transition temperature for the SEB specimen is slightly lower for the 1T SEB specimen in comparison to the 1T CT specimen. This has also been observed in experiments when the transition temperature $T_0$ is evaluated according to ASTM E1921 standard. Hence, the prediction by the model is in line with experimental observation.
Effect of crack depth and specimen size on the fracture toughness transition curve

Experiments have been conducted both shallow-cracked (a/W=0.13) and deeply cracked (a/W=0.53) 1T SEB specimens. The fracture toughness variation in the DBTT regime has been calculated by the model for the shallow-cracked SEB specimen and the results are plotted in Fig. 7 along with experimental data and the master curve data. It can be observed that the FE model has been able to predict the experimental scatter very well in the whole DBTT region. The scatter in fracture toughness as predicted by the model for the deeply cracked specimen has been compared with that of the shallow-cracked specimen in Fig. 8. The fracture toughness values of the shallow-cracked SEB specimen are considerably higher compared to the deeply-cracked SEB specimen and hence, the transition temperature is also lower for the shallow-cracked specimen. Hence, shallow-cracked specimens are less prone to transition compared to deeply-cracked specimens. This is in line with experimental observation.

![Fig. 9: Effect of specimen size on fracture toughness variation in DBTT regime [1T, 2T and 4T CT]](image)

As the crack-tip constraint is lower for the shallow-cracked specimens, the magnitude of crack-tip stress field is lower compared to the deeply-cracked specimens for the same level of loading. This results in lower values of Weibull stresses and hence, the probability of fracture is lower for a given value of K_C loading in case of the shallow-cracked specimen. In components, the cracks present are usually surface cracks with very small depth compared to the thickness and hence, the data of shallow-cracked specimens are more valid for evaluation of transition temperature in these cases. The master curve as evaluated from deeply-cracked specimens cannot be applied directly for safety evaluation of actual components with very small surface cracks and hence, the modelling technique as presented in this work will be very useful for such situations. Similarly, the effect of specimen size on the fracture toughness variation in the DBTT region was also studied. Fig. 9 presents the predicted results for the 1T, 2T and 4T CT specimens. The 2T and 4T CT specimens are scaled versions of 1T CT specimens with scale factors of 2 and 4 respectively. It can be observed from Fig. 9 that the scatter in the fracture toughness decreases for the specimens with larger dimensions, signifying the increase in the fracture toughness transition temperature. Hence, specimens with larger dimensions are more susceptible to the ductile-to-brittle transition for a given value of loading. This is in line with the experimental observations.

![Fig. 10: Material stress-strain data at different temperatures for the pressure vessel steel-2](image)

Prediction of fracture transition curve for the pressure vessel steel material-2

In order to demonstrate the applicability of the model to different materials, a different type of pressure vessel steel is considered here. The composition of the material is similar that of the standard pressure vessel steel of Grade SA508CL2. The stress-strain data at different temperatures for this material is presented in Fig.
Fig. 11 shows the scatter in the experimental data for fracture toughness at different temperatures. The transition temperature $T_0$ has been evaluated as -74 deg. C following ASTM standard procedure. However, when data at different temperatures are considered, different values of $T_0$ has been obtained with a lower bound of -84.9 deg. C and an upper bound of -70.3 deg. C. Analysis is carried out with the mesh-independent damage model and the probability of failure is obtained at different temperatures at different values of loading parameter $K_{JC}$. The predicted data of fracture toughness variation and its scatter with temperature has been plotted along with the experimental data and the data from master curve approach in Fig. 11. The results of the model compares very well with that of experiment. Hence, it can be concluded that the model has been able to satisfactorily model the scatter in fracture toughness in the DBTT region for various types of materials, specimen geometry, size, crack depth and loading conditions etc.

CONCLUSIONS

Analysis of ductile-to-brittle transition temperature $T_0$ is very important for safety analysis of critical components in nuclear and other industries where the material may be subjected to operation in the DBTT regime due to degradation in the material properties due to ageing and other phenomena. It may not possible or economic to conduct experiments with wide variety of specimen geometry, size and loading conditions in order to estimate the transition temperature $T_0$ which is required for application of master curve methodology. In this work, it was demonstrated that a combined nonlocal damage model along with the Beremin’s model can satisfactorily predict the scatter in fracture toughness in the DBTT regime for a wide variety of specimen geometry, size and loading conditions with the use of a single set of Weibull parameters. The parameters of the model are transferable across different specimen geometries and hence, these may be used for a reliable safety analysis of critical components in the DBTT regime of ferritic steels.

REFERENCES