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Prediction of fracture toughness in ductile-to-brittle transition region using combined CDM and Beremin models

Mastaneh Moattari [a], Iradj Sattari-Far [a], Italo Persechino [b], Nicola Bonora [b,*]

[a] Mechanical Engineering Department, Amirkabir University of Technology, PO Box 15875-4413, Tehran, Iran
[b] Civil and Mechanical Engineering Department, University of Cassino and Southern Lazio, I-03043 Cassino, Italy

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ABSTRACT

Scatter of fracture toughness in the ductile-to-brittle transition (DTB) region for ferritic steels may show a dependence on the specimen geometry constraint. Consequently, this can be a source of uncertainty in transferring fracture data from one test geometry to other configurations. In this work, the modified Beremin model (**MBM**) for cleavage and the Bonora damage model (BDM) for ductile tearing, were combined to account for the two failure mechanisms competing in the DTB and to predict fracture toughness scatter band with temperature. The model was validated predicting the scatter in the fracture toughness data of A533B steel for SEB specimens with shallow and deep crack. Present model predictions were compared with master curve results. For the **MBM**, a more physical definition for the process zone was introduced and the temperature dependence of the reference stress σ_u was described by the sum of athermal and thermally activated stress contributions. Results indicate that ductile crack growth occurring before fracture, which is predicted by the ductile damage model, has a relevant effect on the computed probability of brittle fracture. The proposed combined model is able to accurately account for the loss of constraint occurring in different specimen geometries confirming the geometry transferability of model parameters.

1. Introduction

Although FCC metals generally remain ductile at low temperature, BCC metals, such as carbon and low alloy steels, exhibit a change in the fracture mode, from ductile to brittle, as the temperature is decreased over a transition region. This behavior is because, in contrast to FCC metal crystals, the yield stress or critical resolved shear stress of BCC single crystals, is markedly temperature dependent, in particular at low temperatures, as a result of the presence of interstitial impurities and temperature dependent Peierls–Nabarro force. However, the crack propagation stress is relatively independent of temperature. Thus, the mode of failure changes from plastic (ductile) at high temperature to brittle fracture (cleavage) at low temperature. For that reason, the fracture toughness properties of many carbon and low alloy steels can exhibit an excessive amount of data scatter. In the ductile-to-brittle (DTB) transition region, the scatter in the measured fracture toughness values is greatly increased over that normally observed at test temperature either above or below this transition [1]. In this temperature region, some amount of stable (ductile) crack growth can occur, eventually followed by complete fracture by cleavage, indicating that material fracture resistance is the result of the competition between cleavage and ductile rupture [2].

Such loss of stability due to cleavage cannot be explained within the framework of J–R approaches, based on experimentally measured resistance curves at macroscopic scale. In fact, this is caused by a change in the micro-mechanism during fracture, which is also statistical in nature. This behavior is even more marked in the upper transition region as recognized in a large variety of experiments over the years [3].

The scatter observed in the experiments is not only related to the material and its microstructural state [4], but it is also influenced by specimen geometry and crack depth ratio [5]. In fact, the loss of constraint that characterizes different specimen geometries or deep vs shallow crack configurations, contributes to determine the nature of the stress field at the crack tip with effects on both K_{Ic}, in the lower shelf, and on the crack resistance curve, in the upper shelf regime [6].

Fracture mechanics concepts are not based on and do not take into account any specific micromechanism of failure, although the assumptions and requirements for their applicability imply cleavage under limited plastic deformation. Alternatively, "local approaches" and "micromechanical models" address the occurrence

* Corresponding author.
E-mail addresses: m.moattari@aut.ac.ir (M. Moattari), Sattari@aut.ac.ir (I. Sattari-Far), i.persechino@unicas.it (I. Persechino), nbonora@unicas.it (N. Bonora).

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of damage and fracture in materials accounting for specific micromechanisms responsible for rupture. Compared with classical fracture mechanics, the general advantage is that parameters, of the respective models, are only material and not geometry dependent, ensuring transferability from specimen to structure over a wide range of sizes and shape [7].

For what concerns ductile rupture, in the last decades, several models have been proposed. Today, they can be categorized in abrupt criteria [8], void nucleation and growth (NAG) [9,10] and continuum damage mechanics (CDM) [11,12] models which mainly differ for the level of coupling between the specific damage variable and the material constitutive response.

For brittle fracture, Griffith criterion establishes the relationship between the size of a crack and the stress that must be exceeded for the crack to start to grow. Ritchie et al. [13] extended such criterion introducing the additional requirement that the critical stress should be achieved over some microstructurally relevant distance. Curry and Knott [14] proposed a model where cleavage involved a statistical competition between different sized microcracks in the steep stress gradient ahead of the crack. Since 1980, the prevalent criteria for cleavage fracture are based on a "local approach" [15–17]. The majority of the models nowadays, originates from the Beremin-model [15,18], which is a two parameter Weibull model initially intended to predict cleavage fracture in notched samples and later used mainly for application to crack problems. Such type of model is also indicated as weakest link model (WLM) since the cumulative probability of fracture is derived from Weibull statistics under such assumption. A comprehensive description of cleavage fracture models development can be found in [19]. All these models have both advantages and drawbacks. Probably, the major limitations of the Beremin model are an unrealistic treatment of the microcrack population and the lack to account for plastic deformation. Recently, to mitigate the limitations of the Beremin model several modified or improved weakest link based models have been proposed [20–22]. In these models, a number of hypotheses on the mechanisms controlling the nucleation and growth of weak spots eventually responsible for triggering cleavage fracture are made. However, so far, there exists no commonly accepted model that can correctly predict failure for all possible loading conditions and geometries.

The possible use of ductile damage modeling, to simulate ductile crack growth, together with weakest link model was firstly showed by Xia and Shih [23]. Such combination of models showed a potential for application to ductile-to-brittle transition (DTB) region to account for ductile crack growth occurring prior fracture. Ruggieri and Dodds [24] investigated the effect of ductile tearing and constraint on cleavage fracture stress using the Gurson model and WLM. Others followed the same approach. Schmitta, Suna, Bernauer and Nagel [25] used the Gurson model and Weibull stress approach to predict fracture in the transition region on Charpy impact test. Gao et al. [26], based on the experimental fracture data provided by Wallin [27] on 21/4 Cr-1Mo steel, found that the Beremin approach still gives good results if appropriate correction, to account for subcritical crack growth, is made. Later, O'Dowd et al. [28] and Neto and Ruggieri [29] used the Gurson model and the Beremin approach to investigate fracture under small scale yielding conditions. Petti and Dodds [30] investigated the effect of ductile tearing, by means of discrete modeling of microvoids, on cleavage fracture. Esposito et al. [31] showed that increasing temperature, when approaching the nihil ductility temperature (NDT), the identification procedure for local approach parameters breakdown no longer providing a unique set of σ_W and m values.

More Recently, Samalb et al. [32] proposed a combined non-local (mesh independent) ductile damage and cleavage fracture model to predict the fracture toughness transition curve of ferritic steels. Linse and Kuna [33] predicted the values of fracture toughness by numerical simulation of fracture mechanics tests using material parameters identified from the SPT. They used a non-local formulation of a ductile damage model in combination with a modified Beremin model (**MBM**) to characterize the fracture behavior of pressure vessel steels in the transition region. Gehrlicher et al. [34] simulated failure in the transition region coupling the non-local Rousselier (NLR) model and the original Beremin formulation investigating the applicability of NLR model to low stress triaxiality and mixed mode fracture.

A fundamental aspect of ductile rupture, is that stress triaxiality reduces material strain to failure. In different ways, this feature is accounted for in all models addressing ductile failure. In the Gurson model, stress triaxiality amplifies the softening effect on the plastic flow surface associated with porosity accumulation according to an arbitrary assumed function (hyperbolic cosine for the original Gurson model). In CDM, the effect of stress triaxiality on material ductility is obtained, without the need of additional arbitrary assumption, from the definition of the equivalent stress for a damaged material [35] in the framework of thermodynamics of irreversible deformation. The Gurson model showed some limitations in predicting ductile failure for stress triaxiality largely different from that used for model parameters identification. Faleskog et al. [36] found an explicit dependence of the Gurson damage parameters q_1 and q_2 on material hardening exponent and stress triaxiality level. Kim et al. [37] showed that these parameters cannot be treated as universal constants.

Alternatively, the Bonora damage model [38], which is derived in the framework of CDM proposed by Lemaitre [11], has shown a good transferability of the material model parameters over a very wide range of stress triaxiality allowing to predict accurately the constraint effect on the material crack resistance curve [39,40] and CTOD fracture parameter in the upper shelf regime [41].

To investigate the fracture toughness scatter in the DBT region of ferritic steels, Wallin [16,42] proposed the master curve method which is based on the statistical analysis of experimental fracture data assuming a constant temperature dependence for cleavage fracture toughness. The master curve method allows the prediction of the fracture toughness curve in terms of fracture toughness reference temperature (T_0), for any given fracture probability and any specimen thickness, on the basis of small sized specimen testing. In the master curve method, a fracture toughness curve is determined by a single parameter that establishes the position of the master curve on temperature scale. This parameter, indicated as T_0, is defined as the temperature at which the median fracture toughness for 1T-CT fracture toughness specimen equals 100 MPa$\sqrt{m}$ [43]. The master curve introduces a simple empirical relationship that requires a minimum of 6 valid fracture toughness experiments to obtain T_0 for the given specimen geometry and material [44].

Therefore, the possibility to use, a physically-based model that, once calibrated, can provide a prediction of the expected scatter and the geometry effect on the material fracture toughness at different temperatures without the need to perform new experimental tests, would be very useful.

In this work, the Bonora damage model was used coupled with the modified Beremin model to predict fracture resistance of a ferritic steel in the DBT region. At present, possible mutual influence between the two model formulations was neglected.

For the modified Beremin model, a physically sound definition of the process zone, over which the Weibull stress is calculated, was introduced. The coupled model was calibrated on fracture data obtained with standard compact tension (CT) specimen and then validated predicting fracture toughness in single edge notch specimen in bending (SEB) with different crack depths. Predicted scatter in the fracture toughness at different temperature was