An enhanced local approach model for the assessment of brittle fracture based on micromechanical investigations

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Abstract. The objective of the present study is the development of a micromechanically based probabilistic model for the assessment of the cleavage fracture probability of ferritic steels. Brittle fracture of ferritic steels is a probabilistic process, triggered by the failure of randomly distributed brittle particles. These particles fracture due to plastic deformation of the surrounding matrix, resulting in the nucleation of micro-cracks. Once nucleated, the local stress state controls the possible instability of the defects. In this context, the local stress-triaxiality is assumed to govern the blunting of freshly nucleated micro-defects. The local approach models available in literature account for the above-mentioned correlations only in a simplified manner. Based on Representative Volume Elements (RVE) of the microstructure, accounting for the grain-structure as well as for the brittle particles, the cleavage initiation process was modelled in order to investigate the relevant parameters and their interactions. The RVE's were loaded according to the local mechanical field quantities determined numerically for a variety of specimen types at the cleavage-origins. Thus, the behaviour of the particles against the micromechanical conditions could be specified, resulting in a better understanding of the processes at cleavage fracture initiation. Based on the results, an enhanced probabilistic cleavage model is proposed.

Introduction

The brittle fracture of metals is a probabilistic process, triggered by the failure of randomly distributed brittle particles. In this regard, the failure of the particles is caused by plastic deformation of the surrounding matrix [1, 2]. The possible subsequent instability of the nucleated micro defects is governed by the local stress state, in most cases described in terms of the local maximum principal stress σ_1 [3]. An extension of this framework has been proposed by Chen et al. [4], assuming that the nucleation of micro defects is governed by the local accumulated plastic strain ε_e^{pl}, while their possible immediate blunting is controlled by the local stress triaxiality ratio h as a third parameter. Based on this framework, a number of probabilistic models have been proposed in literature. Most of these models are based on the weakest link assumption [5]. The Beremin group [3] proposed a rather simple model using the assumption that all possibly critical micro defects are nucleated at the onset of plastic deformation, so that the cleavage initiation process is purely stress controlled. Further developments include the introduction of a threshold value for cleavage initiation [6] or an incremental formulation [7]. In addition, several alternative models have been proposed, as the recent approach by Faleskog et al. [8], which explicitly includes stress and plastic strain effects.

The present study is concerned with the development of an enhanced probabilistic cleavage fracture model, accounting for the nucleation and the instability of micro defects as well as for the role of the possible blunting of freshly nucleated defects.

Material Characterisation

The material investigated was a German 22NiMoCr3-7 nuclear grade pressure vessel steel. The considered steel exhibits a bainitic microstructure. Especially at the boundaries of the bainitic packets brittle particles can be found, acting as potential cleavage initiation sites. For an appropriate modeling of the RVE's, a statistical characterization of the microstructure (grains and particles) is required. Hence, the material was examined by metallographic methods. In a first step, the microstructure was analysed by means of the electron backscatter diffraction (EBSD) method. Thus, precise information regarding the grain size distribution, the grain shape and the grain orientation (morphologic and crystallographic) were obtained. Based on the morphologic information in the form of best-fit-ellipses, the grain size distribution, the grain shape distribution (ratio of the semi-axes) and the orientation distribution of the grains could be determined. In a second step, a scanning electron microscope (SEM) analysis was performed to specify the size and the shape of the brittle second phase particles acting as potential cleavage initiation sites. Figure 1 shows the Inverse Pole Figure of a typical microstructure and the scanning electron microscope image of the particles.

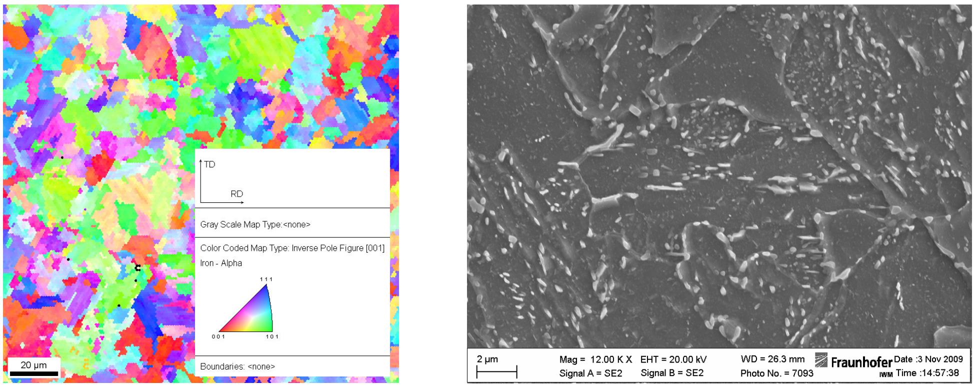

Fig. 1: Inverse Pole Figure of a typical microstructure and SEM-image of the particles

Local Conditions for Cleavage Initiation

As a basis for the development of an enhanced local fracture model, an experimental database from different types of fracture mechanics specimens was available [9, 10]. A fractographic investigation of all tested specimens using scanning electron microscopy provided the fracture mechanism and the position of the cleavage triggering points. In order to investigate the mechanical conditions leading to the initiation of cleavage fracture, all fracture mechanics experiments were analyzed numerically using the finite element method. From the results, the local load histories were extracted at the individual cleavage triggering points. Based on the framework proposed by Chen et al. [4], the maximum principal stress σ_1 is considered as the relevant quantity for instability of existing micro defects, whereas the accumulated plastic strain ε_e^{pl} and the local stress triaxiality ratio $h = \sigma_{kk}/(3\sigma_e)$ are considered as the relevant quantities for nucleation and possible blunting of micro defects. As pointed out in a previous study, the two quantities ε_e^{pl} and h at fracture are interrelated rather than being independent from each other [9]. Cleavage is initiated either during the approach or on a unique failure curve in terms of $\ln \varepsilon_e^{pl}(h(t))$.

The statistical information obtained from the material characterisation enable the generation of statistically representative geometrical models of the grain structure. Based on these geometrical models, finite elements models can be generated using 8-node brick elements. The particles were inserted into the grain structure at the desired location via a spherical submodel, consisting of the material of two adjacent grains and a brittle particle with user-defined size, shape and orientation at the interface of these grains. The submodelling technique enables a very fine mesh of 10-node tetrahedron elements in the vicinity of the particle. The RVE and a submodel are presented in Fig. 2.

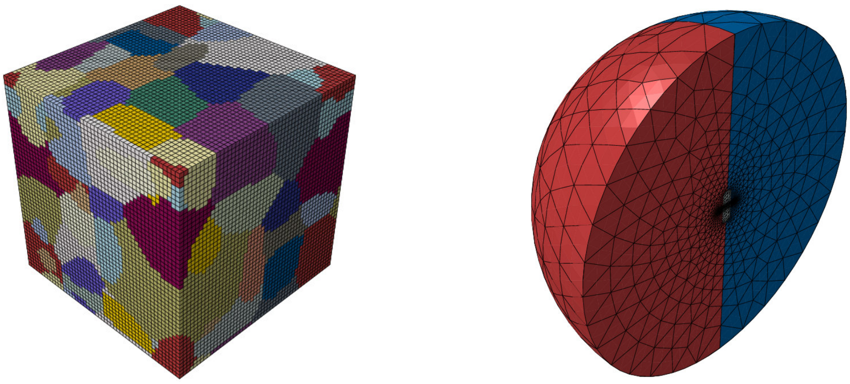

Fig. 2: RVE and submodel (submodel magnified in relation to the RVE)

For the individual grains a single crystal plasticity material model [11] was used, while the particles were modelled as purely elastic. The crystallographic orientation for each grain was determined corresponding to the experimentally calculated misorientation distribution function. Subsequently, periodic boundary conditions were applied and the RVE's could be loaded according to the local load histories obtained from the macroscopic simulations. During the load history, the particle fails when the maximum principle stress is sufficiently high and the total elastic strain energy within the particle reaches a critical value. The formation of an initially sharp micro defect was realised via a node release technique. Subsequently, the behaviour of the micro defect could be considered, e.g. if the defect remains sharp and therefore critical or if the defect blunts and so becomes uncritical with respect to cleavage initiation. Fig. 3 shows the behaviour of a micro defect for different loading conditions. The first load history corresponds to the mechanical fields near a crack front with a low h and a high ε_e^{pl} at micro defect formation, while the second load history represents the mechanical fields near a crack front with a high h and a low ε_e^{pl} at micro defect formation. For both load histories the defect remains sharp, whereas the stress level in the vicinity of the particle is higher for the first load history. Nevertheless, the overall (RVE) stress level is sufficiently high in terms of the Griffith criterion to drive the micro crack in both cases. The influence of the local stress field will be considered in further investigations.

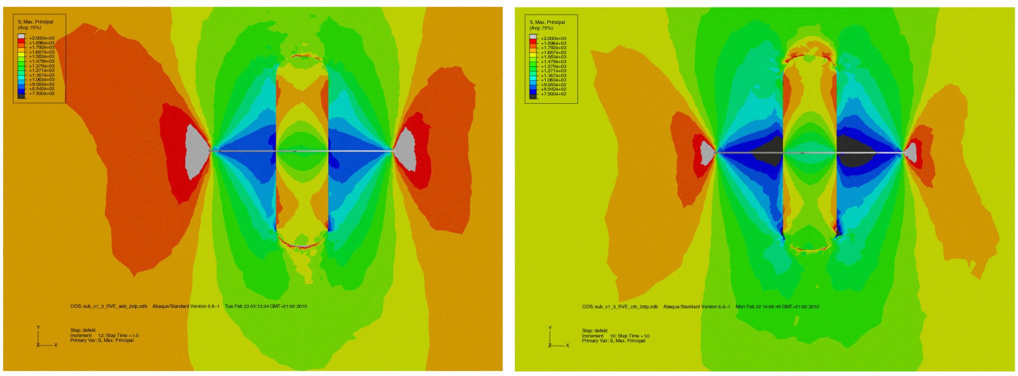

Fig. 3: Particle for different loading conditions

The results of the simulations reveal that a high stress triaxiality ratio increases the probability of formation of potentially critical micro defects.

Enhanced Probabilistic Cleavage Fracture Model

The results on the local conditions for cleavage initiation suggest a two criteria approach for a local assessment of the cleavage initiation probability. While the probability of the instability of existing micro defects is described in terms of the local σ_I, the probability of nucleation of micro defects as the second necessary criterion for cleavage initiation is assumed to be governed by a combination of the local ε_e^{pl} and the local stress triaxiality ratio h. Adopting the framework introduced by Faleskog et al. [8], the probability of failure of the volume element is given by two functions $f_n(\varepsilon_e^{pl}, h)$ and

$f_i(\sigma_1)$ describing the contribution of the nucleation and instability related criteria, respectively. The instability related function is determined in the usual manner by assuming a prescribed statistical size distribution for the existing micro defects in conjunction with the assumption that the instability of existing micro defects is controlled by the Griffith criterion [3, 8]. The nucleation related function $f_n(\varepsilon_e^{pl}, h)$ is assumed to depend on the distance of the state $\ln \varepsilon_e^{pl}(h(t))$ from the failure curve which is approximated by a general linear function in the semi-logarithmic $\ln \varepsilon_e^{pl}$-h diagram. Since it has been shown by Gurland [1] as well as McMahon and Cohen [2] that the number of cracked carbides in ferritic steels increases approximately linearly with increasing macroscopic plastic strain, the dependence of $f_n(\varepsilon_e^{pl}, h)$ on the distance from the failure curve is formulated such that the linear influence of the equivalent plastic strain ε_e^{pl} is recovered. Hence,

$$f_n(\varepsilon_e^{pl}, h) = Ce^{ah}\varepsilon_e^{pl} \tag{1}$$

where C and a are material parameters.

Conclusions

In the present study, the local conditions leading to cleavage initiation were analyzed by finite element simulations on the specimen level as well as on the microstructure level. The results reveal that the instability of existing micro defects is governed by the maximum principal stress whereas a combination of plastic strain and stress triaxiality ratio controls the nucleation of potentially critical micro defects. In this regard, the results of the microstructure simulations support the assumptions of the macroscopically formulated model. Thus, an enhanced probabilistic cleavage fracture model is proposed.

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