Enhancement of local approach models for assessment of cleavage fracture considering micromechanical aspects

Volker Hardenacke[1,a], Jörg Hohe[1,b], Valérie Friedmann[1,c], Dieter Siegele[1,d]

[1] Fraunhofer-Institut für Werkstoffmechanik IWM, Wöhlerstr. 11, 79108 Freiburg, Germany

[a]volker.hardenacke@iwm.fraunhofer.de, [b]joerg.hohe@iwm.fraunhofer.de,

[c]valerie.friedmann@iwm.fraunhofer.de, [d]dieter.siegele@iwm.fraunhofer.de

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Abstract. The objective of the current contribution is the derivation of a micro mechanics based local probabilistic cleavage model for the assessment of the cleavage probability of ferritic steels.
The probabilistic cleavage models available in literature account for the processes on the micro structural level only in a simplified manner. By a micromechanical modelling of the cleavage initiation process the effects and the interactions of the relevant parameters can be identified more precisely. For this purpose Representative Volume Elements (RVE) of the microstructure are considered, accounting for both, the grain structure as well as the brittle particles within the grain structure. The RVE's are loaded based on the local mechanical field quantities at the cleavage origins determined numerically for a variety of deep and shallow crack specimens. Thereby, the behaviour of the brittle particles acting as cleavage initiation sites can be specified for different mechanical loading conditions. By this micromechanical modelling the relevant parameters for the formulation of an enhanced local probabilistic cleavage model are determined.
The model defined in this study accounts for micro defect nucleation as well as for the possible instability of potentially critical micro defects and provides a tool for the integrity assessment in consideration of the local loading conditions.

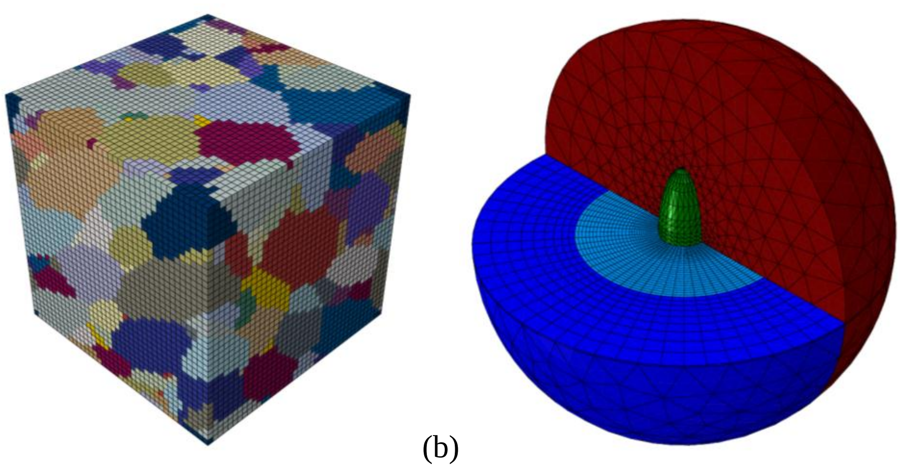
Introduction

The cleavage fracture of bainitic steels is a probabilistic process, triggered by the failure of brittle second phase particles which are preferentially located at grain boundaries. The failure of the brittle particles is a result of the plastic deformation of the surrounding ductile matrix [1,2]. After particle fracture, potentially critical micro cracks may develop if their immediate blunting is constrained by the local stress state [3]. The possible subsequent instability of the potentially critical micro cracks is also governed by the local stress state, in most cases described in terms of the local maximum principal stress σ_I [4]. The instability of a micro crack can cause macroscopic crack initiation if the propagating micro crack overcomes the first barrier, such as a grain boundary.
Considering these mechanisms, various probabilistic models have been proposed in literature. Most of these models are based on the weakest link assumption that the failure of a small volume element triggers the failure of the entire structure [5]. The Beremin group [4] proposed a simple model using the assumption that all potentially critical micro defects are nucleated at the onset of plastic deformation, so that the cleavage initiation process is purely stress controlled. Refined approaches based on the Beremin model include the introduction of a threshold value for cleavage initiation [6] or an incremental formulation [7]. Further developments yielded alternative models that explicitly include stress and plastic strain effects at micro defect nucleation, as the approach by Faleskog et al. [8] or the model proposed by Hohe et al. [9], which also incorporates the effect of stress triaxiality.
The present study is concerned with a refined analysis of the micromechanical basis for the derivation of enhanced cleavage models. For this purpose, the micromechanical processes at micro

defect nucleation are investigated via numerical simulations on the micro structural level using Representative Volume Elements (RVE) of the grain structure and submodels of the grain boundaries. The first part of the investigations includes the examination of the conditions for particle fracture. In this context, the influence of the local field quantities is considered, as well as the experimentally observed effects of particle shape and particle orientation [1,10]. The second part of the investigations deals with the transition of the defect from the broken brittle particle into the surrounding ductile matrix. Thereby, the existing experimental [2,11] and numerical [12] insights concerning this important phase of micro defect nucleation are expanded, resulting in an expression for the critical particle size with respect to defect transition. Based on the results of the simulations and the stochastic description of the microstructure an enhanced cleavage model can be derived.

Micro mechanical simulations

The material investigated is a German 22NiMoCr3-7 nuclear grade pressure vessel steel. The considered material has a bainitic microstructure, with brittle particles located at the boundaries of the bainitic packets. In terms of an appropriate modelling of the RVE's, a statistical characterization of the grain structure and the particles is required. The microstructure was analysed by means of the EBSD method to get information regarding the grain size distribution, the grain shape and the grain orientation (morphologic and crystallographic). Furthermore, a SEM analysis was performed to specify the size and the shape of the brittle second phase particles. Details concerning the material characterization can be found in [13]. Based on the statistical information obtained from the material characterisation and a procedure proposed by St. Pierre et al. [14], finite element models of the grain structure were generated using 8-node brick elements. The particles can be inserted into such a grain structure at the desired grain boundaries using spherical submodels, consisting of the material of two adjacent grains and a brittle particle with the requested size, shape and orientation. The submodelling technique allows a very fine mesh of 10-node tetrahedron elements in the vicinity of the particle. Additionally, a layer of cohesive elements enables the modelling of micro crack propagation within the submodel. Examples for the RVE and a submodel are presented in Fig. 1.

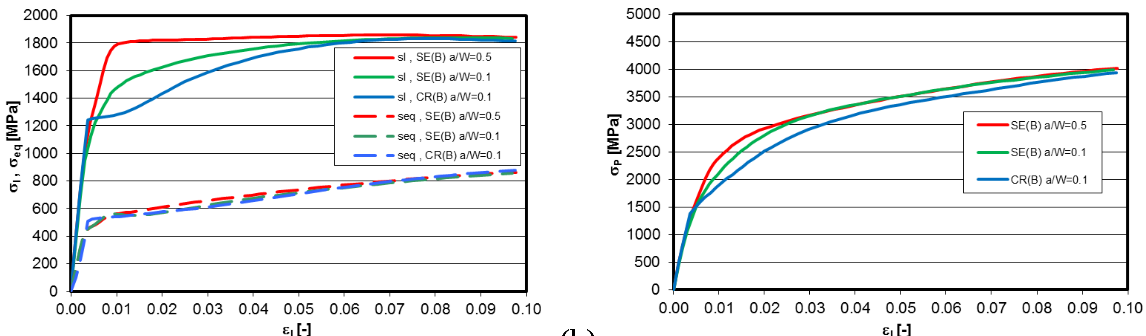


(a) (b)

Fig. 1. (a) RVE (200 grains, edge length 60 μm); (b) Cut through submodel (grain one: blue; grain two: red; diameter 6 μm; cohesive elements: light blue; particle: green)

For the material behaviour of the individual grains a single crystal plasticity material model [15,16] was utilised, in which the crystallographic orientations for the grains were determined corresponding to the experimentally obtained misorientation distribution function. The particles were modelled as purely elastic. After the application of periodic boundary conditions the RVE's were loaded according to typical local load histories at cleavage initiation spots obtained from macroscopic simulations of different fracture mechanics experiments [9].

Particle fracture. Particle fracture as the first phase of cleavage initiation occurs if the maximum principal stress in the particle reaches a critical value. Hence, submodel calculations were performed to identify the influence of the matrix field quantities on the particle stress σ_P. Furthermore, the effects of particle shape and particle orientation were determined.
The influence of the field quantities was analysed for an ellipsoidal particle with a shape factor $s=a/b-1=2.3$ (mean value for the particles in the considered material) and an orientation angle α (angle between the long axis of the particle and the direction of the applied maximum principle stress in the RVE) of 0°. Fig. 2 shows three different matrix load histories (different fracture mechanics specimen types) and the resulting particle stress histories.



(a) (b)

Fig. 2. (a) Different matrix load histories; (b) Resulting particle stress σ_P

It becomes clear that die matrix strain has an essential influence on the particle stress, since the particle stress increases even in the range of nearly constant matrix maximum principle stress. Nevertheless, a description of the particle stress only using the matrix strain is inaccurate. The resulting particle stress for the observed matrix load histories shows distinct differences in those parts of the load history where the matrix maximum principal stress is considerably different. So it seems reasonable to determine an approximate particle stress using a function depending on the matrix strain and the matrix maximum principle stress.
In a real micro structure, the particles exhibit a wide spectrum of shapes and orientations. Therefore, the effects of shape and orientation on the resulting particle stress for a given load history were analysed using adequate submodels. With respect to the shape, particles with different shape factors $s=a/b-1$ were examined, including shape factors from $s=0$ (sphere) to $s=5.7$ (highly elongated ellipsoid). Subsequently, the orientation angle α was varied for the elongated particles ($s>0$), including orientation angles from $\alpha=0°$ to $\alpha=90°$. The determined particle stresses for different particle configurations in terms of shape factor s and orientation angle α are illustrated in Fig. 3.
The results shown in Fig. 3 clarify that the particle shape as well as the particle orientation have a distinct effect on the resulting particle stress for a given load history. Regarding the particle shape, a steep increase of the particle stress can be observed for more elongated particles. An increase of the orientation angle up to a value of approximately 60° causes a decrease of the particle stress, beyond this value there are only minor changes. It has to be mentioned that effects of shape and orientation are correlated. An increase of the orientation angle weakens the influence of the particle shape and a decreasing elongation reduces the effect of the particle orientation. Nevertheless, the qualitative relations are not affected. Based on the results of the simulations, an approximate particle stress can be determined for different matrix load histories and particle configurations.

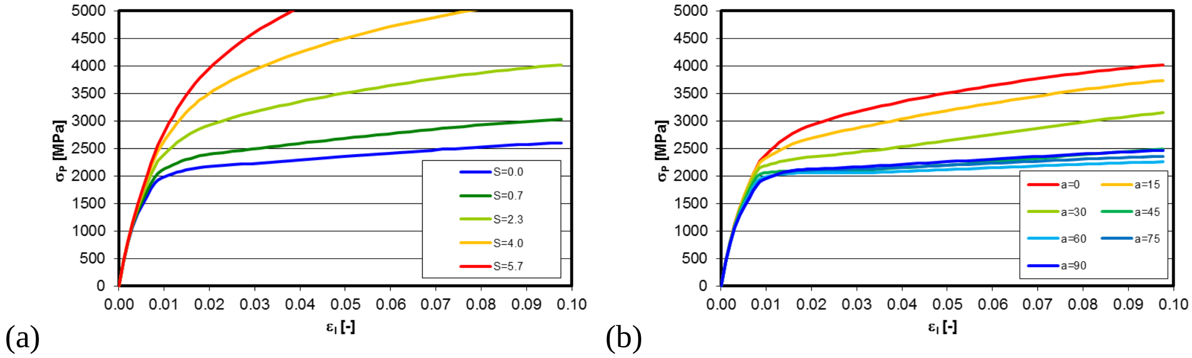


Fig. 3. (a) Effects of shape on σ_P (α=0°); (b) Effects of orientation on σ_P (s=2.3)

Based on the results of the simulations, an approximate particle stress can be determined for different matrix load histories and particle configurations. For this purpose, an appropriate function was defined. This function includes the relevant field quantities (matrix strain and matrix maximum principle stress) and material dependent parameters, which incorporate the effects of the particle configuration (shape, orientation) and the matrix material behaviour.

$$\sigma_P = c_1\sigma_I + c_M c_2 \varepsilon_I^{c_3} \quad (1)$$

with the effective field quantities σ_I and ε_I of the matrix in the vicinity of the particle, the particle configuration dependent parameters $c_i=c_i(s,\alpha)$ (i=1,2,3) and the matrix material dependent parameter c_M, whereas c_i and c_M are not correlated. The particle configuration dependent parameters can be defined for different configurations in the s-α-plane by an adjustment of the particle stress calculated with Eq. 1 to the particle stress from the respective simulation.

Defect transition. The transition of the defect from the brittle particle into the ductile matrix constitutes the second phase of cleavage initiation. Utilising the provided Finite-Element-models, submodel calculations were performed considering different local load histories and particle configurations. The influence of the load history was determined systematically for given particle configurations taking into account all relevant mechanical field quantities. In the first step of the analysis, the behaviour of a spherical particle of constant size was observed for different load histories. A spherical particle provides the advantage that the particle stress exhibits only minor matrixes strain dependence. Hence, the resulting particle stress is very similar for the different applied load histories. Therefore it is possible to analyse only the influence of the mechanical state of the matrix on the process of micro crack propagation. The results of the simulations reveal that the matrix strain has no direct effect with respect to the micro crack propagation. In contrast, the stress state of the matrix exhibits a strong influence on the process of micro crack propagation. A high matrix maximum principal stress and high stress triaxiality promote the transition of the micro defect from the brittle particle into the ductile matrix. For a quantification of the influence of the matrix mechanical state on the transition of the defect, the definition of a critical particle size (diameter in the fracture plane) seems reasonable. The critical particle size D_c specifies the diameter required for a successful transition at a given σ_I-h-state of the matrix. In order to exhibit the critical particle size D_c as a function of matrix maximum principal stress and stress triaxiality, D_c was determined for different states within the σ_I-h –plane. Fig. 4 exemplarily shows the micro defect propagation for different particle diameters at a given matrix stress state. In the case of a diameter lower than the critical particle size D_c, the micro crack arrests immediately after overcoming of the interface of particle and matrix. The stress at the crack front decreases and the micro defect becomes uncritical with respect to cleavage initiation (Fig. 4a). In contrast, for a diameter equal to the critical particle size D_c, no immediate arrest occurs and the micro defect remains critical (Fig. 4b).

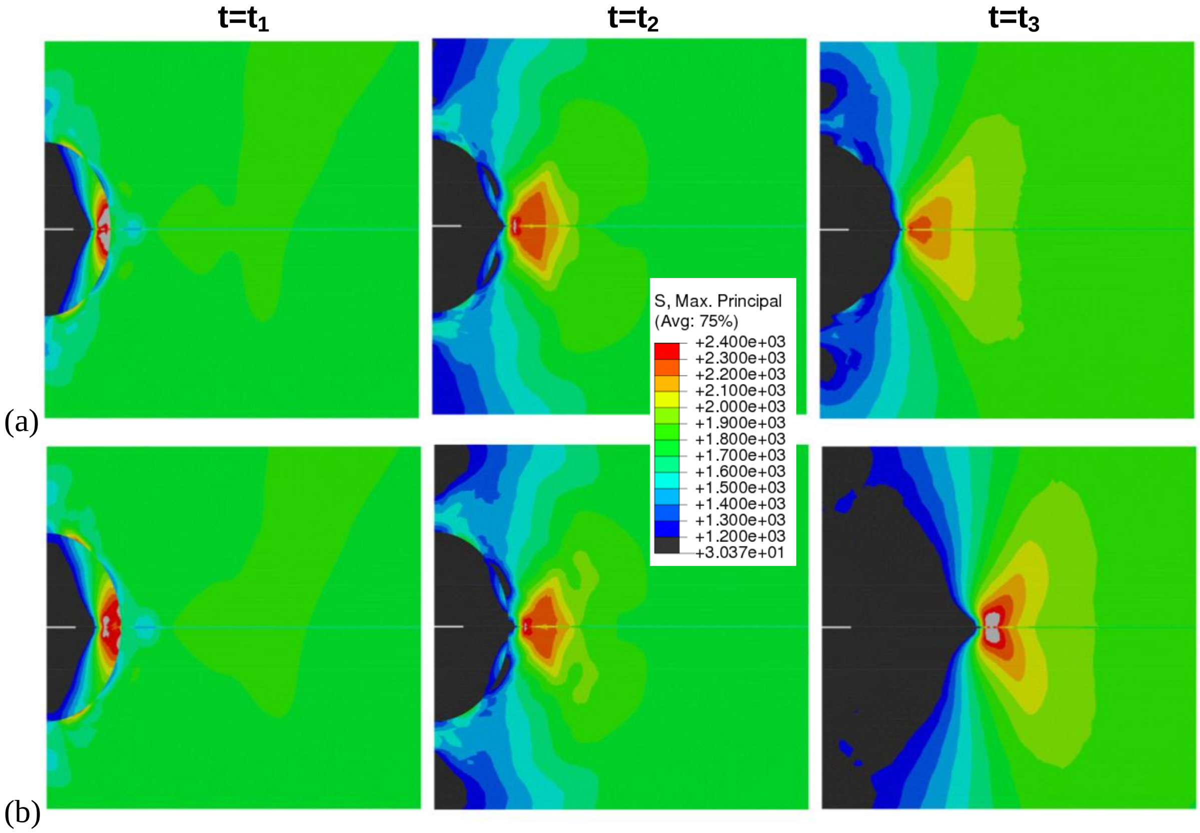


Fig. 4. Micro defect propagation for different particle diameters at a given matrix stress state (contour plot of the maximum principal stress); (a) Particle with $D<D_c$; (b) Particle with $D=D_c$

Further investigations concerning the effect of the particle configuration yielded that the influence of particle shape and orientation can be determined via the particle stress, whereas a higher particle stress reduces the critical particle size.

The results of the simulations reveal that the critical particle size D_c can be determined utilising a function depending on the local matrix maximum principal stress and the local matrix stress triaxiality. Within this function, there must be parameters incorporating the effects of the particle configuration (characterized by the particle stress) and the matrix material behaviour (yield stress, hardening modulus and surface energy). Based on these insights, the critical particle size for a successful transition (no arrest) at a given σ_I-h-state of the matrix is approximately given by

$$D_c = c_1 c_M \sigma_I^{\,c_2} h^{c_3} \qquad (2)$$

with the effective field quantities σ_I and h of the matrix in the vicinity of the particle, the particle configuration (particle stress) dependent parameter $c_1 = c_1(\sigma_P)$ and the matrix material dependent parameter c_M and the constant parameters c_2 and c_3, whereas c_1, c_2, c_3 and c_M are not correlated.

The particle configuration dependent parameter $c_1(\sigma_P)$ can be defined for different states within the σ_I-h-plane by an adjustment of the critical particle size calculated with Eq. 2 to the critical particle size from the respective simulation.

Enhanced local approach model

For the derivation of an enhanced cleavage model we consider a small matrix volume element dV containing brittle particles, which is loaded by the effective stresses σ_{ij} and strains ε_{ij}. The volume element fails if three criteria are fulfilled. The first criterion is related to particle fracture and therefore the particle stress. The second criterion accounts for defect transition and is based on the critical particle size. The possible instability of a nucleated micro defect is assumed to be controlled by the maximum principal stress through a Griffith criterion. This three criteria approach yields the accumulated failure probability of the volume element dV

$$P_f^{dV} = \int_0^t P_{fr}(\varepsilon,\sigma)\, P_{tr}(\sigma,h)\, P_{inst}(\sigma)\, dV\, dt \tag{3}$$

and, utilizing the "weakest-link"-approach [5], the failure probability of the entire structure

$$P_f^{tot} = 1 - e^{-\int_{V^{tot}} P_f^{dV}(dV,t)} \tag{4}$$

Within the separation approach in Eq. 3, the probability for defect instability P_{inst} can be determined in the usual manner from the defect size distribution [4,8]. The probability for particle fracture P_{fr} as well as the probability for defect transition P_{tr} can be determined based on the results of the micromechanical simulations. Eq. 1 and Eq. 2 together with the known stochastic description of the micro structural features (particle shape distribution etc.) enable the computation of the distribution functions for the particle stress and the critical particle size within a volume element for a given effective stress-strain state. Fig. 5 exemplarily shows some of the obtained distribution functions.

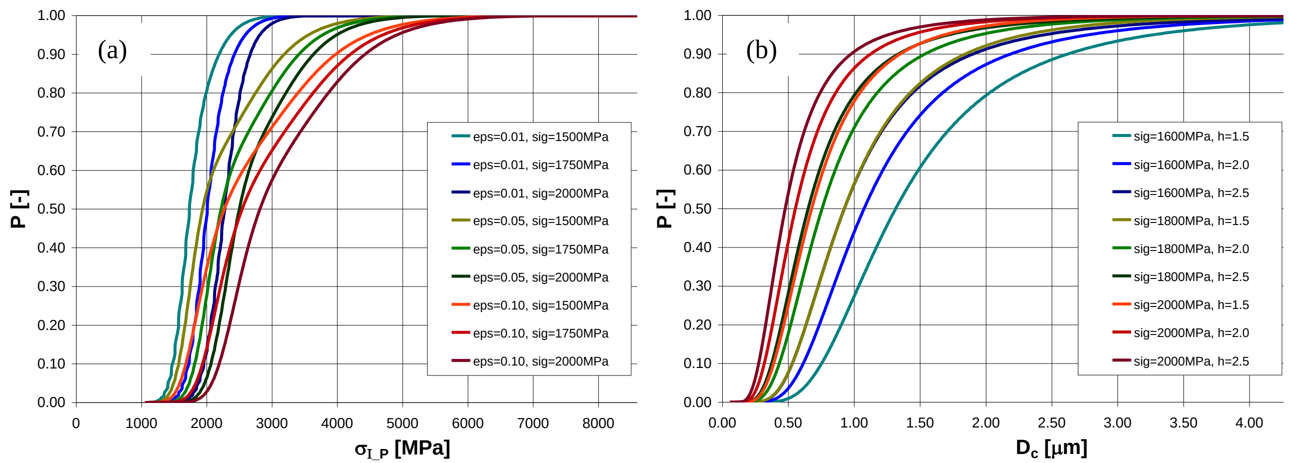


Fig. 4. Distribution functions for different effective stress-strain states of the volume element; (a) particle stress; (b) critical particle size

Approximating the computed distribution functions by three-parameter Weibull-distributions and comparing the distribution function for the particle stress to the particle strength distribution (discrete probabilities w_i^{krit}) and the distribution function for the critical particle size to the particle size distribution (discrete probabilities w_i^{eff}), it is possible to determine P_{fr} and P_{tr}:

$$P_{fr} = \sum_{i=1}^{n} w_i^{krit} \exp\left[-a_S\left(\sigma_i^{krit} - \sigma_0\right)^b\right] \tag{5}$$

$$\sigma_0 = k_1 \varepsilon_I^{k_2} + k_3 \sigma_I \tag{6}$$

$$a_s = k_4 \varepsilon_I^{k_5} \tag{7}$$

$$P_{tr} = \sum_{i=1}^{n} w_i^{eff} \left(1 - \exp\left[-a_{tr}\left(D_i^{eff} - D_0\right)^b\right]\right) \quad (8)$$

$$D_0 = k_6 a_s^{k_7} h^{k_8} \sigma_I^{k_9} \quad (9)$$

$$a_{tr} = [k_{10}(\sigma_0 - k_{11})\exp(-k_{12} a_s) + k_{13} h]\sigma_I^{k_{14}} \quad (10)$$

The parameters k_i are the adaptable model parameters, but only some of them are strongly material dependent.
In a first application, the enhanced model was compared to the Beremin model [4]. The model parameters for both models were fitted for SE(B) fracture mechanics specimens with a/W=0.5 (T = -85°C). Subsequently, the models were applied to determine the fracture probability of SE(B) fracture mechanics specimens with a/W=0.1 (T = -85°C). The results are shown in Fig. 6.

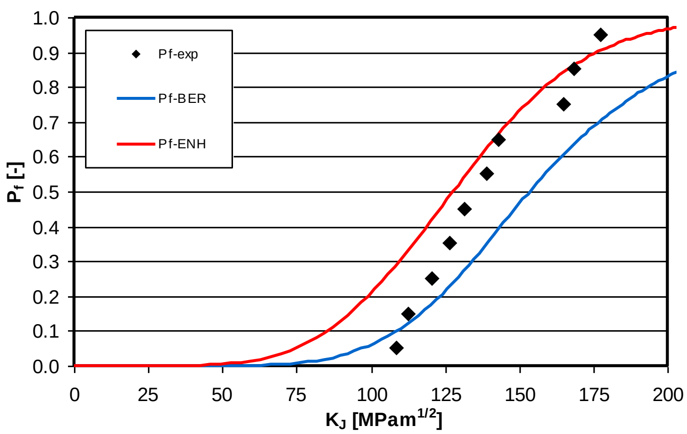


Fig. 6. Comparison of Beremin model and enhanced model

The enhanced model provides a considerably different fracture probability distribution compared to the Beremin model, with an overall improved accuracy.

Conclusions

Within the present study a refined analysis of the micro mechanical basis for probabilistic cleavage models was performed to enable the derivation of an enhanced local approach cleavage model. By a micro mechanical modelling of the cleavage initiation process, based on Representative Volume Elements (RVE) and submodels of the micro structure, the effects and the interactions of the relevant parameters were identified.
In the first step, the process of particle fracture was observed. Assuming that particle fracture occurs if the maximum principal stress within the brittle particle exceeds the respective particle strength, the evolution of the probability for particle fracture can be determined in terms of the existing particle stress. The simulation results reveal that with respect to the local field quantities in the vicinity of the particle the matrix strain ε_I as well as the maximum matrix principal stress σ_I govern the particle stress. In this context, the particle configuration in terms of the particle elongation and the particle orientation (deviation of the long particle axis from the direction of the applied stress) as well as the matrix material behaviour have a strong effect on the resulting particle stress for a given matrix state. In the second step of the investigations, the transition of the defect from the brittle particle into the ductile matrix was observed. The simulation results reveal that with respect to the local field quantities in the vicinity of the particle the matrix stress σ_I as well as the matrix stress

triaxiality *h* govern the critical particle size for a successful transition (no immediate arrest). Besides the matrix stress and the matrix stress triaxiality, the particle configurations in terms of the particle stress as well as the matrix material behaviour affect the critical particle size.
Based on the results of the micromechanical simulations and the stochastic description of the micro structural features an enhanced cleavage model can be derived. The model accounts for micro defect nucleation utilizing the distribution functions of particle stress and critical particle size. In a first application, the enhanced model provides improved results compared to the Beremin model.

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