Micromechanical modeling of crack propagation in nodular cast iron with competing ductile and cleavage failure


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A micromechanical model is employed to simulate the fracture of nodular cast iron in the ductile-brittle transition region. The microstructure is resolved discretely as voids in the process zone. Possible cleavage of the intervoid ligaments is modeled by a cohesive zone. This approach captures both the local fracture stress for cleavage and the energy required to drive the cleavage crack front thus allowing to simulate all stages of crack initiation and propagation in the complete ductile-brittle transition region. A comparison with experiments from literature shows that the model captures the experimental results qualitatively and quantitatively.

Keywords: ductile-brittle transition; micromechanics; finite element analysis; cohesive zone; nodular cast iron

1 Introduction

Due to its excellent grindability, cost-effective production and good strength and toughness properties, nodular cast iron is employed for numerous technical applications, e.g. for gear boxes or nuclear waste casks. The particular values of strength and fracture toughness depend on the active damage mechanism and thus on temperature. In the range of room temperature nodular cast iron fails by a ductile mechanism like most engineering metals: the relatively weakly bonded nodular graphite particles (which typically have a volume fraction of about 10%) debond after low deformations. The thereby created voids grow by plastic deformations and coalesce finally, Figure 1a. The necessary plastic deformations result in a high macroscopic fracture toughness. With decreasing temperature the yield stress increases due to the lower mobility of dislocations. That is why at lower temperatures the local stress level in the microligaments between the voids reaches at some point a critical level whereupon grains with favorably oriented crystallographic planes cleave. Corresponding fracture surfaces are shown in Figure 1b. The cleavage mechanism dissipates considerable less energy and is thus associated with macroscopically brittle behavior. In the ductile-brittle transition region both mechanisms compete as can be seen in Figure 1c.

The loss of fracture toughness associated with the transition from ductile failure to cleavage is a severe problem in many engineering applications. For this reason considerable effort has been dedicated

1The material is also known as “ductile cast iron” (DCI). However, in order to avoid confusion with the damage mechanisms, this term is not used here.
to the development of models for the ductile-brittle transition. Most of these models were developed for ferritic steels. Especially Beremin-type models (Beremin, 1983) are established for evaluating cleavage failure. In this type of models, cleavage initiation is assumed to coincide with complete failure of the structure, the so-called “weakest-link assumption”. However, due to its heterogeneous microstructure, in nodular cast iron macroscopically stable crack propagation by cleavage is observed (Baer, 2014; Ludwig et al., 2012; Pusch, 2008; Pusch et al., 2016; Smirnova and Scheglyuk, 1989). Thus, this material provides a safety reserve which cannot be addressed by the established Beremin-type models. Associated with a macroscopically stable cleavage crack propagation is a lower scatter of the measured fracture toughness values in the ductile-brittle transition region compared e.g. to ferritic steels. Recently, Baer (2014) formulated the following hypothesis as explanation of this behavior of nodular cast iron: “After initiation, the crack propagates by a cleavage mechanism through the small ferritic matrix areas in between the graphite nodules … Each time when the crack runs into the next graphite nodule the crack tip is blunted significantly due to the spheric shape of the particle and it is more or less arrested within a short time. Thus, a number of microscopic pop-ins are superimposed and cause a macroscopic elastic-plastic appearance of the force-time record.”

The aim of the present study is to provide a numerical model that accounts for the individual characteristics of the microstructure of nodular cast iron in the ductile-brittle transition temperature regime allowing to investigate the mechanisms qualitatively and to provide quantitative predictions for the mentioned safety reserve. There are many studies in the literature which deal either with the ductile-brittle transition on the macroscopic scale by Beremin-type models or which resolve the microstructure for the purely ductile mechanism. Reviews on both classes of models can be found in (Pineau, 2006, 2008) and (Benzerga and Leblond, 2010; Tvergaard, 1989), respectively.

However, compared with the large number of papers on these two classes of models, there are relatively few studies where the microstructure and its interaction with cleavage is resolved in a numerical model. To the authors’ knowledge the first models of this type were presented by Tvergaard, Needleman and co-workers (Gao et al., 1996; Needleman and Tvergaard, 1993, 2000; Tvergaard and Needleman, 1988, 1993). These authors modeled the whole domain by the Gurson-Tvergaard-Needleman model (GTN-model) with the microstructure represented by finite regions of nucleable porosity (“islands”). Cleavage is implemented by a node-release technique with a criterion of Ritchie-Knott-Rice-type ("cleavage grains"). However, today it is well-known that constitutive theories within the framework of simple materials (i.e. the current state depends only on the local history of strains) like the GTN-model lead in the softening regime to an ill-posed boundary-value problem. This problem applies also to the “CAFE-model” of Shirenlikht and Howard (2006). Pettit and Dodds (2005) resolve the microstructure in front of the
crack tip discretely in form of a priori existent voids. In general, it is well-known that models with discrete voids within an elastic-plastic matrix predict a plastic collapse and subsequent necking of the intervoid ligaments at sufficient level of loading thus allowing to simulate ductile crack propagation (Hütter et al., 2012; Tvergaard and Hutchinson, 2002). However, Petti and Dods (2005) evaluate possible cleavage only a posteriori locally by means of a Beremin-type criterion, i.e. crack propagation by cleavage cannot be simulated.

A model that allows to model ductile failure and cleavage equivalently in a continuum mechanics consistent way was proposed by Faleskog and co-workers (Kroon and Faleskog, 2005, 2008; Stec and Faleskog, 2009) and Hardenacke et al. (2012). These authors resolved the microstructure in terms of discrete particles and grain boundaries in cell model simulations, i.e. under homogeneous loading conditions, modeling material degradation due to cleavage by a cohesive zone. The latter approach accounts for two main features which are known from experiments: firstly softening due to cleavage initiates when a critical level of the local stress is reached, the cohesive strength. Secondly, the cohesive work of separation corresponds to the fracture toughness of the material for cleavage in absence of plastic deformations. The cohesive work of separation thus forms a minimum fracture toughness for pure cleavage, a feature that is well-known from experiments (see e.g. Anderson et al., 1994).

However, the cell models do not represent the highly inhomogeneous deformations in front of a crack tip adequately. That is why the authors implemented in (Hütter et al., 2014b) a 2D model with discrete voids for the ductile failure and a cohesive zone for cleavage directly in the process zone at the tip of a macroscopic tip. This model allowed to simulate all stages of crack initiation and propagation over the whole ductile-brittle transition region. However, the results gave rise to the suspicion that the geometric representation by a 2D model might be an oversimplification: in a 2D model each intervoid ligament has to be stretched anew until the work-hardening of the metallic matrix lets the local stresses reach the cohesive strength. In contrast, in reality a continuous crack front may form that moves steadily along the crack plane. For this reason, in the present study a more realistic 3D model with spherical voids is used together with cohesive zone for cleavage to model the crack propagation in nodular cast iron in the ductile-brittle transition region.

2 Model

2.1 Global Model

As mentioned already the scope of the present study is to resolve the microstructure at the crack tip discretely to model crack propagation. For the considered nodular cast iron this concerns the graphite nodules. These graphite nodules are relatively weakly bonded to the embedding metallic matrix and can thus be modeled adequately as a priori existent spherical voids. The matrix material is described by Mises plasticity with isotropic hardening. As mentioned already, it is well known from numerous studies in the literature that after some void growth the reduction of the stress-carrying cross section overcompensates the strain-hardening thus leading to macroscopic softening. That is why no further ingredients than a Mises-plastic matrix and discrete voids are necessary to model ductile crack propagation, the mechanism of plastic collapse and necking is sufficient.

But of course in a numerical model the microstructure cannot be resolved discretely in a complete specimen since such a model could not be handled on existing computers. Anyway, it is even not necessary to resolve the microstructure everywhere. Only directly in the process zone at the crack tip gradients occur over distances which are of the same magnitude as the characteristic length of the microstructure, i.e. to the distance $X_0$ of the voids. However, preliminary studies of the purely ductile mechanism (Hütter et al., 2012, 2013) showed that void growth in the plastic zone outside the immediate process zone must nevertheless not be neglected. Although possibly of low magnitude, the void growth in the plastic zone shields the process zone from high triaxial stresses thus retarding at least the ductile fracture initiation. In order to capture this effect possible void growth in the plastic
zone is incorporated in a homogenized way by means of the established GTN-model with the same initial void volume fraction \( f_0 \) as in the discrete process zone. Of course, the effective elastic properties \( E_{\text{eff}} \) and \( \nu_{\text{eff}} \) of the homogenized region have to be determined from the corresponding values \( E \) and \( \nu \) of the matrix incorporating the effect of the voids, too.

\[ r \gg X_0 \]

Figure 2: Semi-infinite crack under mode-I-loading with discrete microstructure and cohesive zone

Figure 3: Exponential cohesive law

In a real material like nodular cast iron the graphite particles are distributed more or less randomly in the matrix with respect to size and location. If one would like to incorporate this distribution in a model one would have to have sufficient information on the statistics of size and location of the graphite nodules. Although costly, such information can be gained in principle. However, using stochastically distributed voids in a model would require firstly to simulate sufficient realizations. Secondly, the process zone where the voids are to be resolved would have to be large enough in thickness direction to be representative. Both measures would increase the numerical effort dramatically, if an implementation would be possible at all. For this reason we investigated in a preliminary study (Hütter et al., 2013) several regular void arrangements in the purely ductile regime. In this case a thin and periodic “slice” has to be implemented in an FE-simulation only. It turned out that the computed crack growth resistance curves (so-called \( R \)-curves) of the regular arrangements for purely ductile behavior form reasonable bounds of corresponding experimental data. Especially the body-centered cubic (bcc) arrangement with crack propagation in the (110) plane in ⟨110⟩ direction recovers the mean \( R \)-curve in the ductile regime quite well. Since the present model for the ductile-brittle transition shall contain of course the purely ductile case, this bcc-arrangement is employed here, too. From the same preliminary study, the definition of the mean void distance as

\[ X_0 = \frac{1}{\sqrt{N_V}} \]  

is adopted as it is applicable both to regular and real stochastic void arrangements, the latter being important for a comparison with experimental data. Therein, \( N_V \) denotes the mean number of voids per volume.

The material parameters for the ductile behavior of nodular cast iron are taken from (Kuna and Sun, 1996). In this study an initial void volume fraction of \( f_0 = 0.113 \) was extracted for the nodular cast iron EN-GJS-400. Performing cell model simulations, Kuna and Sun (1996) calibrated the GTN parameters to \( q_1 = 1.3, q_2 = 0.7, q_3 = q_1^2 \) for this material. In (Hütter et al., 2013) it was found that the measured yield curve \( \bar{\sigma}(\bar{\varepsilon}) \) of the ferritic matrix can be very well fitted by the one-parametric power law that is
used in many of the cited studies. This relation (matrix yield stress $\bar{\sigma}$ as function of the equivalent plastic strain $\bar{\varepsilon}$) is defined implicitly by

$$\frac{\bar{\sigma}}{\sigma_0} = \left( \frac{\bar{\sigma}}{\sigma_0} + \frac{E}{\sigma_0} \right)^N .$$

Therein, $\sigma_0$ and $N$ denote the initial yield stress and the hardening exponent, respectively. Power law (2) is consistently used both for the Mises-matrix in the discrete process zone and for the GTN-model in the homogenized region. The fitted values $\sigma_0/E = 1/900$, $N = 0.20$ are adopted in the present study. The Poisson ratio of the matrix is set to $\nu = 0.3$. Well-known formulas yield for the particular $f_0$ effective (i.e. homogenized) elastic properties of $E_{\text{eff}} = 0.797 E$ and $\nu_{\text{eff}} = 0.287$, respectively (for details see forward [Hütter et al., 2013]).

In order to exclude possible effects of the geometry of a particular specimen, the limiting case of a semi-infinite crack under mode-I-loading and (macroscopic) plane strain conditions is considered as in several of the cited numerical studies. This approach ensures small-scale yielding conditions per se and the state in the process zone is determined uniquely only by the (history of the) far-field stress intensity factor $K_1$. Thus, the $J$-integral corresponds to the far-field energy-release rate $J = K_1^2/E_{\text{eff}}$ where $E_{\text{eff}} = E_{\text{eff}}/(1 - \nu_{\text{eff}}^2)$ denotes the homogenized Young’s modulus under plane strains. Cleavage is modeled by a cohesive zone as explained in the introduction (section 1). In previous studies [Hütter et al., 2011, 2014b] with a cohesive zone embedded in elastic-plastic material we found that local instabilities of snap-through type (so-called pop-ins) may be predicted under some conditions. In addition, according to the discussion in section 1 local pop-ins may be particularly relevant for the ductile-brittle transition of nodular cast iron. That is why the present model needs to incorporate dynamic effects by including the inertia terms. The whole model is sketched in figure 2.

2.2 Cohesive Zone

The established exponential traction-separation law by [Xu and Needleman, 1993] is employed for the cohesive zone in the modification by [Roth et al., 2014] as depicted in figure 3. In form of non-coinciding loading and unloading paths, this modification accounts for the irreversible character of the material degradation by cleavage quantifying it by a damage variable $0 \leq D \leq 1$. This damage variable $D$ is defined as ratio between the dissipated work and the cohesive work of separation $I_0$ as area under the exponential traction separation envelope $t = \sigma_c \delta / \delta_0 e^{1-\delta/\delta_0}$ [Roth et al., 2014]. Thereby, the cohesive strength $\sigma_c$ forms the maximum traction that can be transmitted by the cohesive zone. In the considered case of mode-I-loading, the maximum principal stress appears normal to the crack plane and coincides with the tractions $t$ transmitted by the cohesive zone. Employing a cohesive zone with $\sigma_c$ as maximum transmittable traction corresponds thus to a maximum principle stress criterion, an established and validated approach for cleavage since [Orowan, 1949]. In the present implementation the traction-separation law is formulated with respect to the current configuration, i.e. $\sigma_c$ corresponds to the maximum true stress at cleavage.

A dimensional analysis, as performed e.g. by [Tvergaard and Hutchinson, 2002], shows that the present model (figure 2) can predict only crack growth resistance curves in the form

$$\frac{J}{X_0 \sigma_0} = \text{function} \left( \frac{\Delta a}{X_0}, f_0, \frac{\sigma_0}{E}, N, \frac{\sigma_c}{\sigma_0}, \frac{I_0}{\sigma_0 X_0} \right).$$

Thereby, the ratio $\Delta a/X_0$ is an outcome of the simulations. The influence of the dimensionless parameters $f_0, \sigma_0/E$ and $N$ was investigated in previous studies. In the present study their values are chosen according to experimental data for nodular cast iron as described in section 2.1. Thus, it remains open to investigate the effect of the normalized cohesive properties $\sigma_c/\sigma_0$ and $I_0/(\sigma_0 X_0)$ systematically.

It is clear that the ratio of cohesive strength $\sigma_c$ and matrix yield stress $\sigma_0$ determines which damage mechanism becomes active. If $\sigma_c$ is low compared to $\sigma_0$, then the crack will proceed only due to the
softening in the cohesive zone without any plastic deformations and thus without any void growth, i.e. only by cleavage. In contrast, if \( \sigma_c \) is considerably larger than \( \sigma_0 \), strong plastic deformations are required until the work-hardening drives the local stress level to \( \sigma_c \) corresponding thus to the ductile regime. In this context it has to be remarked that with the present model final failure of an intervoid ligament will appear always in the cohesive zone due to the employed non-saturating hardening law \( \dot{\sigma} \). Thus, in the simulations single values of the damage \( D \) in the cohesive zone cannot be related to ductility. Rather, such information can only be gained from extracted \( R \)-curves which contain the plastic contribution to the dissipation during crack growth.

Regarding the temperature dependence of the quantities \( \sigma_c \) and \( \sigma_0 \), it can firstly be stated that nodular cast iron exhibits an increasing yield stress \( \sigma_0 \) with decreasing temperature as typical engineering metals do. In contrast, it was found already in the beginning of the 1970s (Grifiths and Owen 1971; Knot 1973) that the cleavage fracture stress of mild steels is practically constant over a very wide temperature range. The matrix of mild steels is similar to the considered nodular cast iron so that the cohesive strength \( \sigma_c \) can be assumed to be constant. Thus, the ratio \( \sigma_c/\sigma_0 \) increases with the temperature and the transition to brittle failure with decreasing temperature is mainly driven by the increasing yield stress. In the following simulations the ratio \( \sigma_c/\sigma_0 \) is varied systematically to investigate the influence of temperature.

The cohesive work of separation \( I_0 \) represents the lower-bound fracture toughness for pure cleavage as already discussed. However, the practical determination of this value requires considerable experimental effort. An extensive experimental investigation of the fracture toughness of nodular cast iron in the ductile-brittle transition region for temperatures down to \(-140\,^\circ\text{C}\) was performed by Motz et al. (1980). They found no fracture toughness values (in terms of the stress intensity factor) below \( K_c \approx 1000\,\text{MPa mm}^{1/2} \). This lower-bound fracture toughness corresponds to a work of separation of about \( I_0 = 5\,\text{N mm}^{-1} \). Eq. (3) shows that for the present model the normalized work of separation \( I_0/(\sigma_0 X_0) \) is important. For the ferritic nodular cast iron to be considered later for a comparison with experimental data realistic values of the distance of voids and of the yield stress are \( X_0 = 30\,\mu\text{m} \) to \( 130\,\mu\text{m} \) and \( \sigma_0 = 250\,\text{MPa} \) to \( 300\,\text{MPa} \), respectively. Thus, the normalized work of separation lies in the range \( 0.1 < I_0/(\sigma_0 X_0) < 0.6 \). Out of this range we consider arbitrarily the values \( I_0/(\sigma_0 X_0) = 0.125 \) and \( I_0/(\sigma_0 X_0) = 0.250 \) for the following simulations. Focusing on the temperature dependence by varying the ratio \( \sigma_c/\sigma_0 \), the results in section 3 will refer to \( I_0/(\sigma_0 X_0) = 0.125 \) if not stated otherwise.

### 2.3 Numerical Implementation

Within a finite element implementation of the described model a periodic “slice” of the regular void arrangement has to be meshed. Due to the mode-I-loading only a half model needs to be considered. The mesh that is used in the process zone is shown in figure 4 from two perspectives. The front and back faces \( z = \text{const} \) are fixed to ensure macroscopic plane strain conditions. Due to the regular void arrangement, these boundary conditions coincide with conditions of periodicity and mirror symmetry. Several layers of discrete voids (i.e. in planes parallel to the crack plane) have to be incorporated in the process zone where inhomogeneous deformations of the individual unit cells appear that cannot be described adequately by the GTN-model (Hutter et al. 2012, 2013). Of course the strongest deformations appear in the void layer in the crack plane which is why a fine mesh is required there. The mesh resolution can be reduced in the next layers of voids (figure 4). The coarse and the fine meshed layers are coupled by geometric constraints (“hanging nodes”). In total, the discrete process zone encompasses 7.5 layers each with 16 unit cells in direction of crack propagation. A small initial radius \( r_1 \) is introduced at the initial crack tip to account for crack tip blunting.

The discrete process zone is coupled to the homogenized region by geometric constraints, too. The homogenized region is implemented as a semi-circle of radius \( A_0 = 11,000 \, X_0 \). This size is large compared to the maximum extent of the plastic zone ensuring small-scale yielding conditions. The \( K_1 \)-solution is prescribed as displacement boundary condition at the outer radius \( r = A_0 \).

As discussed in sections 2.2 and 2.3 local pop-ins are expected to occur. In order to deal with such
Figure 4: Mesh in the process zone with cohesive elements from two perspectives

The simulations are performed with the commercial finite element code Abaqus Standard. Hexahedral elements with quadratic shape functions are employed for both the discrete and the homogenized region. The cohesive elements with quadratic shape functions are implemented as user-defined elements via the UEL interface of Abaqus (Roth et al., 2014). They do not have a geometrical thickness but are inserted in Figure 4 only for illustration purposes. Regarding the mesh resolution it can firstly be stated that due to the cohesive zone and the purely geometric softening during the ductile mechanism the boundary value problem is well-posed and a mesh-independent solution is reached asymptotically with decreasing element size. However, this implies vice versa that the minimum mesh resolution that is required in the intervoid ligaments is determined by the cohesive zone. In particular, the length of that part of the cohesive zone where softening appears scales with the intrinsic length that is contained within the cohesive work of separation $\Gamma_0$. This zone of softening needs to be resolved by the FE mesh so that the maximum allowed element size scales also with $\Gamma_0$. The mesh shown in figure 4 employs elements of edge length $b_e = 0.03$ to $0.06 \times X_0$ and is used for the simulations with $\Gamma_0 = 0.250 \sigma_0 X_0$. The simulations with $\Gamma_0 = 0.125 \sigma_0 X_0$ require an even finer mesh (not shown here) with $b_e = 0.015$ to $0.03 \times X_0$. Such a simulation has a nodal degree of freedom of about 1.5 million and requires between 1500 and 3000 time increments. The simulations allow a high degree of parallelization and take in total between 500 and 1000 CPU hours each.

3 Results

The evolutions of the material degradation $D$ due to cleavage and the void growth in the crack plane with increasing far-field loading $J$ are shown in figure 5 for a particular ratio of cohesive strength and yield stress of $\sigma_c/\sigma_0 = 6.7$. In the figure the results of the FE model are mirrored and continued periodically according to the exploited symmetries for illustration purposes. Figure 5a shows that after an initial stage of crack tip blunting, the first voids in front of the initial crack tip have grown considerably by plastic deformations before cleavage initiates indicated by an increase of the damage.
variable $D$ of the cohesive zone. Cleavage does not initiate directly at the initial crack tip but in some distance to it where the voids act as further stress concentrators. Subsequently, a cleavage crack front is formed along the whole thickness direction as shown in figure 5b. Note that the cleavage initiation is instable resulting in a dynamic process as can be seen from the constant level $J = 1.01 \sigma_0 X_0$ of the macroscopic load in figures 5a and 5b. From its initial location the local cleavage crack front propagates already between the first voids although it is not consolidated with the initial crack front over the whole thickness yet. Between the voids the cleavage crack front propagates in a V-shape, a phenomenon that is known from fracture experiments on the macroscopic scale as “tunneling”. When the local cleavage crack front has microscopically tunneled the first intervoid ligament it splits up and runs around the next void as can be seen in figure 5c. In the “shadow” of the first void, the crack fronts reunify within an relatively diffuse zone. Finally, this mechanism repeats, see figure 5d. Figure 5c shows also that the voids in front of the cleavage crack front have grown considerably indicating the competition between the ductile mechanism and cleavage.

As explained already, the competition between both mechanisms is mainly influenced by the ratio of cohesive strength $\sigma_c$ and yield stress $\sigma_0$. In particular, it was discussed in section 2.2 that the ratio corresponds directly to the temperature. The influence of $\sigma_c/\sigma_0$ on the deformations in the process zone is visualized in figure 6a (making again use of the symmetries utilized for the FEM model). In the ductile regime, i.e., for a high ratio $\sigma_c/\sigma_0$, in figure 6a the voids behind the current crack tip have grown significantly leaving only narrow intervoid ligaments on the fracture surface. Note also the waviness (i.e., the non-uniform remanent displacements normal to the crack plane) of the fracture surface in the wake behind the current crack tip which can be attributed to the different local constraint of the plastic deformations due to the presence of the voids. For $\sigma_c/\sigma_0 = 5.5$ in the transition region in figure 6b there are still significant plastic deformations before cleavage occurs (as can be seen best by comparing the remanent widths and heights of the first intervoid ligaments on the front plane). For low temperature in figure 6c, i.e., low $\sigma_c/\sigma_0$, the crack propagates without any significant void growth.

For the envisaged comparison with experimental results, corresponding macroscopic characteristics shall be extracted from the performed simulations, in particular the fracture initiation toughness $J_c$ and the crack growth resistance curves $J(\Delta a)$. This requires practicable definitions of the quantities $J_c$ and $\Delta a$. Finding definitions which apply independent of the active damage mechanism is not trivial for
experiments and thus it is neither for the present simulations which shall recover these experiments. For instance, the amount of crack growth $\Delta a$, which actually represents a mean value of the complex damage zone, cannot be determined by the usual unloading technique in the considered case of ideal small-scale yielding. That is why the definitions of (Hütter et al., 2014b) are adopted: $J_c$ is defined as the kink in the initially linear $J$ vs. CTOD curve indicating the deviation from pure crack tip blunting (Gu, 2000). The crack growth $\Delta a$ is measured from the initial crack tip to the center of the currently active damage zone. Thereby, the center is computed via the location of the individual intervoid ligaments weighted by their necking relative to the final necking far behind the active damage zone. For details of the definitions we refer to the cited publications.

The influence of the ratio of cohesive strength $\sigma_c$ and yield stress $\sigma_0$ on the computed fracture initiation toughness $J_c$ is shown in figure 7 for both investigated parameter sets of the cleavage fracture toughness $I_0$ (relative to void distance $X_0$ and yield stress $\sigma_0$). Both curves exhibit the expected S-

The weighting with the final relative necking leads to a distortion of the blunting line. This distortion influences the extracted $R_c$-curves only near the blunting regime. Nevertheless, in the present study we correct this distortion since the $\Delta a$ from experiments that we want to compare our results finally with lie in this regime.
normalized plot in figure 7. However, practically the upper ductile-brittle transition region is typically of more interest.

Extracted crack growth resistance curves are shown in figure 8 for different values of $\sigma_c/\sigma_0$ exhibiting again the ductile-brittle transition. Firstly, it is found that all $R$-curves increase monotonically, i.e. the crack propagation remains macroscopically stable despite the locally unstable initiation of cleavage as discussed above. This was also the case for the parameter sets not shown in figure 8.

Furthermore, figure 8 shows that both the fracture initiation toughness and the tearing modulus increase with increasing $\sigma_c/\sigma_0$ reaching the $R$-curve for an ideal ductile matrix material asymptotically for $\sigma_c/\sigma_0 \rightarrow \infty$. Practically, the latter limiting case corresponds to a model without a cohesive zone (compare Hütter et al., 2013). Note that figure 7 indicates for $I_0/(X_0\sigma_0) = 0.125$ a saturation in the fracture initiation toughness for $\sigma_c/\sigma_0 \gtrsim 6.5$. Comparing the $R$-curves for $\sigma_c/\sigma_0 = 6.7$ and $\sigma_c/\sigma_0 = 7.9$ in figure 8 confirms this finding. However, despite the minor influence on the fracture initiation toughness, the increase of ductility of the matrix material when going from $\sigma_c/\sigma_0 = 6.7$ to $\sigma_c/\sigma_0 = 7.9$ has a significant influence on the tearing behavior.

In addition, figure 8 shows that the ideally ductile $R$-curve forms an upper limit for all values of cohesive strength. This physically plausible behavior was, though, not observed in a preliminary study with a similar model but with 2D circular voids as discussed in section 2.2. Thus, the present results confirm the hypothesis that the predicted fracture mechanisms of 2D and 3D models are qualitatively different: In a 2D model the intervoid ligaments cleave one after one whereas in the more realistic 3D model a continuous zone of material degradation due to cleavage is formed and propagates along the matrix, figure 5.

4 Comparison with Experiments

Qualitatively, it can firstly be stated that the predicted macroscopically stable crack propagation in the ductile-brittle transition region corresponds to experimental findings as cited in section 1. The present numerical study confirms the hypothesis of Baer (2014) that although macroscopically stable, cleavage initiation leads on the microscale to locally dynamically propagating cracks which arrest at the next void (formed by a debonded graphite particle). In addition, the S-shaped fracture initiation toughness curves as in figure 7 are well known from experiments.

For a quantitative comparison we use the experimental data of Ludwig et al. (2012) for the nodular cast iron EN-GJS-400. By means of the method outlined in Hütter et al. (2013), we obtained a mean distance of the graphite particles of $X_0 = 113 \mu m$ from the micrographs. The macroscopic 0.2% offset yield stress is given as $R_{p0.2} = 246 MPa$ at $20^\circ C$ and $R_{p0.2} = 276 MPa$ at $-40^\circ C$. No values for $R_{p0.2}$ were published between $20^\circ C$ and $-40^\circ C$ which is why the necessary values are interpolated linearly within this range. With these values, the experimental data of Ludwig et al. (2012) are plotted in figure 9 in normalized form.

As open parameters of the present model we have thus only the cohesive properties $\sigma_c$ and $I_0$ which are related to the cleavage of the ferritic matrix. As discussed in section 2.2, the work of separation $I_0$ corresponds to the lower-bound fracture toughness of the matrix. The results in section 3 showed that the ideally ductile matrix $\sigma_c/\sigma_0 \rightarrow \infty$ forms an upper limit of the (normalized) $R$-curves. That is why the ideally ductile $R$-curve from figure 8 is inserted in figure 9 first. For a consistent normalization the relation between initial yield stress $\sigma_0$ of the matrix and the macroscopic offset yield stress $R_{p0.2}$ is required. With the employed hardening parameters and $f_0$, the GTN model yields $\sigma_0 = 1.04 R_{p0.2}$.

Figure 9 shows firstly that the ideally ductile $R$-curve matches the experimental data for $20^\circ C$ quite well (compare Hütter et al., 2013). This indicates that we have a chance to identify suitable values of $\sigma_c$ and $I_0$ that allow us to describe the ductile-brittle transition at all. The experimental data in Ludwig et al. (2012) are not sufficient to identify the lower bound cleavage fracture toughness $I_0$. However, in section 2.2 we referenced corresponding data from literature for a similar material. Together with the relatively large distance $X_0 = 113 \mu m$ of graphite particles for the material of Ludwig et al. (2012),
assuming a ratio \( I_0/(\sigma_0 X_0) = 0.125 \) is justified based on the estimates in section 2.2. The cohesive strength \( \sigma_c \) (corresponding to the local cleavage fracture stress and being temperature-independent as outlined also in section 2.2) is then determined by a parameter fitting. Even the experimental data for \(-40^\circ\)C in figure 9 are not too far away from the ideally ductile curve giving a hint on the range of the ratio \( \sigma_c/\sigma_0 \) we have to focus on. Independent of the actual value of \( \sigma_c \), it can be stated that the ratio \( \sigma_c/\sigma_0 \) decreases by about 12% when going from \(20^\circ\)C to \(-40^\circ\)C just due to the change of \( R_{p0.2} \) and thus of \( \sigma_0 \). With this finding we have selected some computed \( R \)-curves that cover a similar range of \( \sigma_c/\sigma_0 \) in the upper ductile-brittle transition region. Comparing now all computed curves with the experimental results shows a principal agreement. Knowing now the absolute values of \( R_{p0.2} \) and thus of \( \sigma_0 \) allows to identify a cohesive strength of \( \sigma_c \approx 1900 \) MPa.

Although in principal an agreement between the predictions of the present model and the experimental results has been found, it shall not be forgotten that the ideally ductile \( R \)-curve is necessary in figure 9 to cover the range of measured points. This means that actually the model underestimates the effect of the temperature slightly. However, we think that this point is attributed to two effects that are not incorporated in the model yet. Firstly, the cohesive work of separation \( I_0 \), that represents the lower-bound cleavage fracture toughness of the matrix, was assumed to be temperature independent. So the (very extensive) Euro Fracture data set (Heerens and Hellmann, 2002) exhibits a drop of the lower-bound fracture toughness of at least 50% for a temperature decrease of 40K in the upper ductile-brittle transition region. Having a look on figure 7 this means that with decreasing temperature and thus with decreasing \( \sigma_c/\sigma_0 \) we would come from the blue curve to the red one, i.e. actually ductile-brittle transition would appear within a narrower range of the ratio \( \sigma_c/\sigma_0 \). Secondly, Ludwig et al. (2012) used increased rates of loading in order to trigger cleavage. However, the published values \( R_{p0.2} \) were recorded at lower rates of loading thus underestimating the relevant value of the fracture experiment. Regarding the normalized plot in figure 9 this means that the actual normalized \( R \)-curves would lie at a slightly lower level, i.e. in a region where the present model predicts also a higher sensitivity with respect to changes of \( \sigma_c/\sigma_0 \). Thus, the already reasonable predictions of the present model could still be improved if both effects were incorporated. Unfortunately, corresponding experimental data are not available yet.

5 Summary and Outlook

In the present study a micromechanical model is employed to simulate the fracture of nodular cast iron in the ductile-brittle transition region. The weakly bonded graphite particles are idealized to a priori
existing spherical voids that are resolved discretely in the process zone at the crack tip. Possible void
growth around the process zone is incorporated in a homogenized way by means of the GTN-model.
Cleavage is modeled by a cohesive zone capturing both the local fracture stress for cleavage by the
cohesive strength and the energy required to drive the cleavage by the cohesive work of separation.
Investigating a regular void arrangement, it is sufficient to mesh a periodic slice of the configuration in
the finite element implementation thus keeping the numerical effort at a handleable level. A parameter
study is performed with respect to the cohesive parameters. The results showed that the present model
captures qualitatively the behavior of nodular cast iron: the typical S-shape in the fracture initiation
toughness plotted versus the temperature with a well-defined lower-shelf toughness and the stable crack
propagation by cleavage in the ductile-brittle transition region. A comparison with experimental data
from literature demonstrated that the proposed model allows in principle also quantitative predictions
of the fracture initiation and propagation in nodular cast iron. Remarkably, the results of the present
study differ qualitatively from those of a preliminary study with a similar but two-dimensional model.
Thus, it has to be concluded that the computationally more expensive three-dimensional models are
necessary for simulating the ductile-brittle transition adequately on the microscopic level. Presumably,
this conclusion holds also if the ductile failure competes with other damage mechanisms like growth of
secondary voids.

In the present model the plastic behavior of the metallic matrix material was assumed to be rate-
independent in order to keep the number of model parameters as small as possible. However, in practice
the ductile-brittle transition under dynamic loading is a very important topic. So the next step would
be to extend the present model towards rate-dependent behavior. Under dynamic loading conditions,
the competition between strain-rate hardening and adiabatic softening in the intervoid ligaments will
become an interesting aspect. It will also be interesting to apply the present model to other materials
like steel. In steels the fracture initiation by cleavage is, in contrast to nodular cast iron, typically
unstable. Compared to nodular cast iron the void nucleating particles in steels have a lower volume
fraction and are harder than the graphite. So it remains open to investigate the roles of the volume
fraction of particles as well as of their bulk and bonding properties on the ductile-brittle transition.

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**References**


