Dislocation pile-up and cleavage: Effects of strain gradient plasticity on micro-crack initiation in ferritic steel

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Abstract

Micro-cracks in ferritic steel often originate from broken or debonded carbide particles, or from cleavage of the ferrite matrix. Experiments in literature show that dislocation pile-ups at grain boundaries or particles predominantly induce micro-cracks in ferritic steel. On the other hand, the ferrite can also arrest nucleated micro-cracks owing to local plastic deformations which reduce the stresses at the crack tip. In the present study, the competition between these mechanisms is investigated by cell model simulations using effective gradient plasticity (scalar gradient plasticity) for the ferrite. This theory allows to model the dislocation pile-up by suitable interface conditions. Potential cleavage of the ferrite or failure of the carbide is modelled by a cohesive zone. Parameter studies are performed with respect to the size of the particle and the strengths of ferrite and carbide.

Keywords: Ferritic steel, Gradient plasticity, Unit cell model, Ductile-brittle transition

1 Introduction

Ferritic steels exhibit a ductile to brittle transition at low temperatures and/or high rates of deformation. The associated loss of toughness is critical in many engineering applications. The brittle behavior is related to transgranular cleavage of the ferrite \[1\]. It is well-known that microstructural features of ferritic steel have a strong influence on fracture toughness. There are two main types of particles in ferritic steel at microscopic scale: non-metallic inclusions (manganese sulfides and oxides, which often have large sizes) and carbide particles (so-called carbides) \[2\]. In particular, the cementite particles ($\text{Fe}_3\text{C}$) are a major factor for fracture of ferritic steel in the ductile-to-brittle transition regime. This applies especially to modern pressure vessel steels containing a reduced amount of sulfur so that the effect of MnS inclusions as failure site (origin) is reduced \[3\]. Kroon, Faleskog and coauthors \[4-6\] proposed a micromechanics approach in which an elastic-plastic constitutive law is used for the deformation of ferrite together with a cohesive zone model for three failure mechanisms, namely cracking and debonding of carbide as well as for potential cleavage of the ferrite. A unit cell model with pre-cracked carbide embedded in the ferrite was employed. The major objective of their research was to investigate the fibre-loading mechanism and the influence of stress triaxiality as well as plastic strain rate (i.e., indirectly related to the change of temperature) on micro-crack initiation. However, their
model could not account for the local stress amplifications at grain boundaries due to a pile-up of dislocations, although it is known that this so-called strengthening mechanism is important to initiate micro-cracks in ferritic steel [7]. The pile-up of dislocations can be described on the continuum mechanics level only with gradient plasticity theories. In the present study, the unit cell concept is adopted together with an effective gradient plasticity approach to investigate the interaction between pile-ups of dislocations, at carbide-ferrite interface and grain boundaries, and the nucleation of cleavage micro-cracks.

2 Effective gradient plasticity

2.1 Formulation

Numerous gradient plasticity theories have been proposed in literature. Higher order theories follow Mindlin’s strain gradient theory in which higher order stresses are defined as the work conjugate of strain gradients in the energy potential [8-11]. For a review, refer to [12]. Higher order theories are formulated within a thermodynamic framework and require additional boundary conditions. On the other hand, low order theories introduce gradient dependencies directly into the yield condition [13-16]. Consequently, low order theories do not require additional boundary conditions. For that reason, they reduce the complexity compared to higher order theories. Low order strain gradient theories can be implemented in finite element analysis with the conventional framework of \( J_2 \) plasticity.

The effective plastic strain gradient was firstly proposed by Aifantis [17]. In this model, the second gradient of equivalent plastic strain \( \varepsilon^p \) was incorporated in the yield function. This model is considered a special case of Fleck and Hutchinson’s model [18], which is referred to as ‘explicit’ gradient enhancement. In order to solve this problem in finite element analysis, it requires \( C^4 \) continuity [19]. Therefore, the implementation of this model in finite element analysis is quite difficult. To overcome this difficulty, Peerlings [20] proposed an ‘implicit’ gradient formulation. It involves a non-local counterpart \( \dot{\varepsilon}^p \) to the equivalent plastic strain \( \varepsilon^p \) together with the spatial gradient \( \nabla \dot{\varepsilon}^p \). This model only requires \( C^0 \) continuity. With its single additional nodal degree of freedom, it is attractive for the implementation into the finite element framework. The model involves a Mises-type yield function

\[
f = \sigma_e - \sigma_f \tag{1}
\]

with a flow stress

\[
\sigma_f = \sigma_y (\varepsilon^p) + \frac{3}{2} \hat{h} (\varepsilon^p - \dot{\varepsilon}^p)
\]

and

\[
\sigma_e = \sqrt{\frac{3}{2} \sigma'_{ij} \sigma'_{ij}}, \quad \varepsilon^p = \sqrt{\frac{2}{3} \varepsilon_{ij} \varepsilon_{ij}}
\]

together with the micro-force balance

\[
\dot{\varepsilon}^p - \varepsilon^p = \ell^2 \nabla^2 \dot{\varepsilon}^p. \tag{2}
\]

Therein, \( \sigma_e \) is the von Mises equivalent stress and \( \sigma_y (\varepsilon^p) \) refers to the yield curve under homogeneous deformations. As non-classical stress and \( \sigma_y (\varepsilon^p) \) appears as an intrinsic material length scale in front of the Laplace operator \( \nabla^2 \). Furthermore, an additional parameter \( \hat{h} \) is required which penalizes the difference between \( \varepsilon^p \) and \( \dot{\varepsilon}^p \). Equation (2) needs to be accompanied by suitable boundary conditions. This can be a micro-hard boundary \( \dot{\varepsilon}^p = 0 \) or a micro-free boundary \( \vec{n} \cdot \nabla \dot{\varepsilon}^p = 0 \).
2.2 Relation to dislocation densities

It is commonly assumed the flow stress $\sigma_f$ correlates to the densities of statistically stored dislocations (SSDs) and geometrically necessary dislocations (GNDs). SSDs are created in the lattice by trapping each other in random ways while the structure is imposed to homogeneous plastic deformation. The random patterns of SSDs are relevant under homogeneous plastic deformations, whereas GNDs ensure compatibility under non-uniform plastic deformation, e.g. at grain boundaries. Both types of dislocations contribute to the strain hardening.

Within the effective plastic strain gradient model under consideration, the densities $\rho_S$ and $\rho_G$ of SSDs and GNDs are related to the equivalent plastic strain $\varepsilon^p$ and its gradient $\nabla \varepsilon^p$ [21], respectively. The total density of dislocation amounts to $\rho_T = \rho_S + \rho_G$. Different approaches have been proposed for the individual contributions of $\rho_G$ and $\rho_S$ to the hardening. In the present study, the model by Abu Al-Rub and coauthors [22-25] is employed for the interpretation of the finite-element results with respect to dislocation densities in a post-processing step. The model is based on the critical flow stress concept introduced by Columbus and Grujicic [26]:

$$\sigma_f = \left[\sigma_S^\beta + \sigma_G^\beta\right]^{1/\beta}.$$  \hspace{1cm} (3)

Therein, $\beta$ is an interaction coefficient. Furthermore, $\sigma_G$ and $\sigma_S$ are the flow stresses associated with the densities $\rho_G$ and $\rho_S$, respectively, which can be expressed through Taylor hardening law as

$$\sigma_G = m \alpha G b \sqrt{\rho_G}, \quad \sigma_S = m \alpha G b \sqrt{\rho_S} \tag{4}$$

wherein $m$ is the Taylor factor, $G$ is the shear modulus, $b$ is the magnitude of the Burgers vector and $\alpha$ refers to an empirical coefficient ($\alpha = 0.1 \ldots 0.5$) [25, 27, 28].

Consequently, the flow stress as a functions of the dislocation densities reads

$$\sigma_f = m \alpha G b \left[\rho_S^{\beta/2} + \rho_G^{\beta/2}\right]^{1/\beta} \tag{5}.$$ 

This equation shows the contributions of the densities of SSDs and GNDs on the strain hardening. For $\beta = 1$, Eq. (5) has the same structure as Eq. (1) of the present gradient model, i.e. the flow stress comprises two additive terms, associated with homogeneous (SSD) and inhomogeneous (GND) contributions. If both equations are evaluated firstly for a uniform state of deformation, i.e. $\nabla^2 \varepsilon^p = 0$ (corresponding to $\dot{\varepsilon}^p = \varepsilon^p$), and secondly for a non-uniform deformation, the densities of both types of dislocations can be identified as

$$\rho_S = \left(\frac{\sigma_f (\varepsilon^p)}{m \alpha G b}\right)^2, \quad \rho_G = \left(\frac{h \varepsilon^p}{G} \frac{\ell^2 \nabla^2 \varepsilon^p}{m \alpha b}\right)^2 = \left(\frac{h \varepsilon^p}{G} - \varepsilon^p \right)^2 \frac{\ell^2 \nabla^2 \varepsilon^p}{m \alpha b}. \tag{6}$$

Regarding the present model of gradient plasticity, the application of Eq. (6) is a post-processing step whereby the product $m \alpha b$ acts as a scaling factor.

2.3 Numerical implementation

In the context of gradient-enriched damage models, Seupel et al. [29] pointed out that the micro-force balance [2] has the same structure as a stationary heat equation $c\nabla^2 T + r = 0$. 

3
Consequently, the implementation effort can be reduced drastically by using built-in thermo-mechanical elements in a thermomechanically coupled analysis of the commercial FEM code Abaqus/Standard [30] if the temperature is identified as $T = \dot{\varepsilon}^p$. The heat capacity needs to be chosen as $c = \ell^2$. The heat source is set to $r = \dot{\varepsilon}^p - \varepsilon^p$ by means of the HETVAL user subroutine. Finally, the effective yield stress $\sigma_f$ in the yield condition, Eq. (1), needs to be set to $\sigma_f = \sigma_y (\varepsilon^p) + \frac{3}{2} \cdot h \cdot (\varepsilon^p - \dot{\varepsilon}^p)$ by means of the UHARD user subroutine which has access to the temperature field $T = \dot{\varepsilon}^p$. This user subroutine is provided as supplementary material.

In the envisaged application, the crack propagation may become unstable which requires a dynamic analysis. Unfortunately, Abaqus/Standard does not support inertia effects in thermomechanically coupled analyses. In the modified Newmark method, the inertia terms give rise to additional nodal forces (similar to d’Alembert forces). These dynamic nodal forces can be added to a thermomechanically coupled analysis in Abaqus/standard as described in the Appendix.

2.4 Verification

In order to verify the implementation, the problem of simple shearing of a strip of height $H$ is used as a benchmark. The strip is assumed to have an infinite length in $x$ direction. The boundary conditions are sketched in Figure 1. Note that micro-hard boundary conditions $\dot{\varepsilon}^p = 0$ are prescribed at the bottom and the top surface. Since the strip has infinite length, both sides of the finite width layer $W$ in the FE model are periodically constrained. In the verification step, the material of the layer is simply assumed to exhibit linear isotropic strain hardening

$$\sigma_y(\varepsilon^p) = \sigma_0 + h \varepsilon^p$$

(7)

wherein $\sigma_0$ is the initial yield stress and $h$ refers to the hardening modulus.

Material properties are chosen as in [31]: $\sigma_0 = G/100$, $h = 20 \sigma_0$, $h = 2 G/3$. The ratio $H/l$ between height and intrinsic length is varied.

Under simple shear loading, the solution of the boundary-value problem for the infinite strip can be found analytically by solving the ODE

$$\frac{d^2 \dot{\varepsilon}^p}{dy^2} - \lambda^2 \cdot \dot{\varepsilon}^p + \frac{\sqrt{3} \sigma_{12} - \sigma_0}{\beta} = 0 \quad \text{with} \quad \lambda^2 = \frac{h}{\ell^2 \left( h + \frac{3}{2} h \right)}$$

(8)

for the non-local equivalent plastic strain. For micro-hard boundary conditions, the solution

Figure 1: Simple shear of the infinite layer with boundary conditions
\[ \tilde{\varepsilon}_p = \sqrt{3}\sigma_{12} - \sigma_0 \frac{1 - \cosh(y\lambda)}{\cosh(H/2)} \]  

Consequently, the relation between shear stress \( \sigma_{12} \) (which is constant in the layer) and mean shearing \( \Gamma = U/H \) is obtained as

\[ \sigma_{12} = G \left( \Gamma + \frac{\sqrt{3} \sigma_0}{h} \left[ 1 - \frac{3h}{h + \frac{3h}{2}} \tanh(\frac{\lambda H}{2}) \right] \right) \left( 1 + \frac{3G}{h} \left[ 1 - \frac{3h}{h + \frac{3h}{2}} \tanh(\frac{\lambda H}{2}) \right] \right). \]  

The analytical solution and FEM simulation of the shear stress \( \sigma_{12} \) (normalized with initial shear stress \( \tau_0 = \sigma_0/\sqrt{3} \)) and mean shear strain \( \Gamma \) are given in Figure 2(a) for different ratios of height to internal length scale \( H/\ell \). The distribution of equivalent plastic strain across the height of the layer is plotted in Figure 2(b). In both figures, the FEM solution coincides obviously with the analytical solution so that the presented FEM implementation is verified.

### 3 Micromechanical Model

#### 3.1 Cell model

An axi-symmetric unit cell model under uni-axial macroscopic loading is adopted to investigate the interaction between pile-ups of dislocations with the initiation of cleavage micro-cracks as shown schematically in Figure 3. The cell encompasses a spherical carbide particle embedded into two grains of ferrite. Potential fracture of the ferrite by cleavage or of the carbide and the interface between both is modeled by cohesive zones. Cleavage of ferrite or of the carbide is assumed to appear only along the plane of symmetry \( z = 0 \). Therefore, only a quarter of the cell needs to be incorporated in the finite element analysis. The dimensions of the cell model are chosen as \( H_0 = R_0 = 7.45R \) (corresponding to a volume fraction of carbide \( V_p = 0.16\% \)). A uniform vertical displacement \( U_z \) is applied at the top surface \( z = H_0 \). The outer surface \( r = R_0 \) is assumed to remain cylindrical but without resulting radial loading, compare e.g.
Figure 3: Axi-symmetric unit cell model under uniaxial loading

[32] Regarding the plasticity model, micro-free boundary conditions are applied at the outer surface of the unit cell. The influence of the respective jump conditions at the interfaces is investigated below in section 4.1.

The load is applied quasi-statically, i.e., slow enough that inertia effects are negligible when the cracks propagate stably. This means that the load is applied within a time \( \tau_L \) which is much longer than the time \( \tau_{wave} = R_0/c_R \) that the elastic waves need to pass the characteristic distance \( R \) of the problem (\( c_R \) is the velocity of the slower Rayleigh waves). In particular, \( \tau_{wave}/\tau_L = 0.001 \) is chosen in the simulations, using the same values of mass density for ferrite and carbide [4].

Quadrilateral elements with bi-linear shape functions and reduced integration (CAX8RT in the library of Abaqus) are used for the FEM simulations. The element size \( L_e \) amounts to \( L_e = 0.02 R \) in the regions of the cohesive zones. For the employed parameter sets, this choice ensures that the element size remains comparable to the intrinsic length \( \delta_0 \) of the cohesive zone \( L_e \leq 1.25\delta_0 \). The mesh is coarsened towards the upper parts of the cell model as shown in Figure 3.

3.2 Cohesive zone model

The cohesive zone model developed by Roth [33] is used for three types of potential failure (carbide cracking, debonding of carbide-ferrite interface and cleavage in the ferrite). Under monotonous loading, the traction-separation relation follows an exponential curve

\[
 t = \sigma_c \frac{\delta}{\delta_0} \exp \left(1 - \frac{\delta}{\delta_0} \right).
\]  

(11)
However, beyond the maximum transmittable stress at $\delta = \delta_0$, called the cohesive strength $\sigma_c$, the unloading path towards the origin deviates from Eq. (11). This behavior represents dissipation of energy during the separation process as illustrated in Figure 4. For the FEM analyses, the cohesive zone is implemented in Abaqus/Standard as a user-defined element via the UEL subroutine [33].

The two parameters of the cohesive law, i.e. the cohesive work of separation $\Gamma_0$ and the cohesive strength $\sigma_c$, are named corresponding to three types of modes of failure: $\Gamma_{0M}$, $\Gamma_{0P}$ and $\Gamma_{0PM}$ are the cohesive work of separation of ferritic matrix, carbide particle and for the debonding of carbide-ferrite interface, respectively. Analogously, $\sigma_{cM}$, $\sigma_{cP}$ and $\sigma_{cPM}$ are the cohesive strengths of the ferritic matrix, carbide and carbide-ferrite interface, respectively. Actually, it is quite difficult to define exact values of these parameters. That is why the values $\Gamma_{0PM} = \Gamma_{0M}$ and $\Gamma_{0P} = 0.5\Gamma_{0M}$ from literature [46, 34, 35] are adopted here. The cohesive strengths are chosen as $\sigma_{cP} = \sigma_{cPM} \leq \sigma_{cM}$ [35].

Regarding the temperature dependence of the ferritic steel mentioned in [4, 5], it is well-known that $\sigma_c$ is hardly dependent on temperature. In contrast, the yield stress $\sigma_0$ of the ferrite increases with decreasing temperature [36]. Consequently, the ratio $\sigma_c/\sigma_0$ increases with increasing temperature and $\sigma_c/\sigma_0$ decreases with decreasing temperature [37]. A parameter study is performed with respect to the ratio $\sigma_c/\sigma_0$, which also implies indirectly the influence of temperature on the fracture mechanism in the considered microstructure.

3.3 Material parameters

The isotropic hardening curve $\sigma_y(\varepsilon_P)$ of the ferrite is given implicitly by

$$\frac{\sigma_y}{\sigma_0} = \left(\frac{\sigma_y}{\sigma_0} + \frac{E}{\sigma_0} \varepsilon_P\right)^N.$$  \hspace{1cm} (12)

Therein, $E$ is Young’s modulus and $N$ is the hardening exponent. Such a relation gives rise to a power-law with respect to the total strain under uni-axial loading, compare e.g. [37].

The penalty parameter of the effective plastic strain gradient is adopted from [19] as $h = 10h_0$, wherein $h_0 = \frac{NE}{h}$ is the initial modulus of the power law hardening. The intrinsic material length scale $\ell$ can be determined from indentation tests [7, 38]. The value of this quantity is assumed to lie in the $\mu$m range [29], i.e. of similar magnitude as the size of the carbide particles.
Table 1: Material properties for the cell model [36, 40]

<table>
<thead>
<tr>
<th>Material</th>
<th>$E/\sigma_0$</th>
<th>$\nu$</th>
<th>$N$</th>
<th>$\ell/R$</th>
<th>$\sigma_c/\sigma_0$</th>
<th>$\Gamma_0/(\sigma_0 R)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ferrite (the matrix)</td>
<td>333</td>
<td>0.3</td>
<td>0.1</td>
<td>0...0.8</td>
<td>1...12</td>
<td>1.05</td>
</tr>
<tr>
<td>Carbide</td>
<td>666</td>
<td>0.3</td>
<td>-</td>
<td>-</td>
<td>0.1...12</td>
<td>0.625</td>
</tr>
<tr>
<td>Carbide-ferrite interface</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.1...12</td>
<td>1.05</td>
</tr>
</tbody>
</table>

For dimensional reasons, the ratio $\ell/R$ of both quantities is relevant for the plasticity-related size-effect of the present model. The particular influence of the ratio $\ell/R$ will be investigated within a parameter study.

The material properties used for the cell model are given in Tab. 1. Therein, the values of the work of separation of a carbide particle, the interface and matrix, respectively, are normalized to the carbide size $R$ and the initial yield strength (i. e. $\Gamma/(\sigma_0 R)$).

4 Results and discussion

4.1 Influence of micro-hard boundary conditions, internal length scale and grain size

Firstly, the effect of the non-classical boundary and jump conditions of the scalar gradient plasticity theory shall be investigated. For this purpose, micro-hard conditions ($\dot{\varepsilon}^p|_{\text{interface}} = 0$) are applied to the grain boundary (GB) or along the circumference of the particle (PB), respectively. Figure 5a shows the effective, macroscopic stress strain curves $\Sigma_z - E_z$ of the unit cell simulations. Typical failure mechanisms and the distribution of the maximum principal stress $\sigma_I$ are illustrated in Figure 5b. It can be seen that when micro-hard conditions are applied neither at the particle circumference nor at the grain boundary (case 2) or only at the particle circumference (case 3), the computed stress-strain curve does not exhibit significant differences compared to the simulations with classical plasticity (case 1). Obviously, the dislocation pile-up at the particle is hardly relevant to the macroscopic strain hardening. However, if the micro-hard condition is applied only at the grain boundary (case 4), strain hardening increases
significantly until a micro-crack initiates at the grain boundary. When the micro-crack reaches the particle-matrix interface, it triggers debonding of the particle from the matrix. In the last case (case 5⃝), micro-hard conditions are applied to both the grain boundary and to the particle interface. In this case, the particle breaks after the initial micro-crack arrives at the particle-matrix interface. The stress-strain curves are similar for both cases (case 4⃝ and case 5⃝), but the micro-crack mechanisms in the cell model are significantly different. In following sections, micro-hard conditions are applied on both, the grain boundary and the particle circumference, for all simulations.

The intrinsic length scale parameter \( \ell \) can be considered as a bridge between plasticity at micro-scale and plasticity at macro-scale. The gradient effects vanish and the conventional plasticity theory is recovered if the characteristic length is set equal to zero \( \ell = 0 \). Figure 6 illustrates the effect of the gradient plasticity compared with the conventional plasticity theory. It shows that the incorporation of gradient effects, i.e. non-vanishing values of \( \ell / R \), induces a higher initial hardening which leads to initiation of cleavage at lower levels of macroscopic strain \( E_z \). For large values \( \ell / R \geq 0.6 \), i.e., for small carbides \( R \) or a low density of dislocations, the initiation of cleavage leads immediately to a complete failure and the macroscopic stress \( \Sigma_z \) drops to zero. However, for lower values of \( \ell / R \), the cleavage microcrack can be arrested. For a smaller value \( \ell / R = 0.2 \), even three distinct stages are observed: Firstly, maximum principal stress concentrates at the grain boundary due to dislocation pile-up (stage 1⃝). When the principal stress exceeds cohesive strength \( \sigma_{cM} \) of the matrix, a micro-crack initiates at the grain boundary (stage 2⃝). Subsequently, the crack grows into both grains. The dissipation due to the plastic deformations at the tips of the growing microcrack leads to a limited macroscopic hardening (stage 3⃝). When the microcrack arrives at the carbide, the latter debonds and the macroscopic stress drops again (stage 4⃝). Further loading is necessary to drive the right tip of the microcrack through the elastic-plastic second grain (stage 5⃝). Finally, the crack propagates dynamically through the ligament of the second, carbide-free grain until complete separation of the material occurs (stage 6⃝).

A real material contains a population of carbides of different size. The intrinsic length \( \ell \) is a characteristic of micro-plastic deformation, i.e. dislocation processes in the ferritic matrix, and therefore considered a constant property. Then, Figure 6 indicates that cleavage will initiate near the largest carbides, since initiation there requires the lowest level of the macroscopic strain.
For a given total volume fraction of carbides, the microstructure can differ with respect to the distance $R_{g1} - R$ of the carbide to the next grain boundary, compare Figure 3. In order to investigate this influence, the ratio $R_{g1}/R$ is varied. In this context it has to be remarked that the ratio $R_{g1}/R$ determines also the volume fraction of the carbide within the respective grain and that distance of the carbide to the grain boundary and its volume fraction in the grain cannot be varied independently in the present axi-symmetric model. The simulation results in Figure 7 show that the macroscopic strength, the hardening behavior as well as the crack arrest capability depend strongly on $R_{g1}/R$, i.e., on the distance of the carbide to the grain boundary. In particular, a lower ratio $R_{g1}/R$ leads to a lower strength, but requires a larger amount of dissipation for driving the micro-crack. Furthermore, the microscopic failure mechanism depends on $R_{g1}/R$: if the carbide is located close to the grain boundary $R_{g1}/R = 2.5$, the particle breaks before cleavage initiates in the matrix. This prediction complies with the experimental finding that carbides close to or at a grain boundary are prone to initiate cleavage. The transition point with respect to $R_{g1}/R$ between micro-crack initiation in the carbide and in the matrix depends on the strength of particle and matrix (not shown here).

In following sections, the internal length and the the size of the grain with carbide are chosen at intermediate levels $\ell/R = 0.4$ and $R_{g1}/R = 3.75$, respectively.

4.2 Influence of cohesive strength on micro-crack mechanisms

The influences of the strengths of the particle-matrix interface $\sigma_{cPM}$ and of the matrix $\sigma_{cM}$ shall be investigated by means of sensitivity studies. The (normalized) strength of the particle-matrix interface $\sigma_{cPM}/\sigma_0$ is varied in the range of $0.1 \ldots 12$ and that of ferrite $\sigma_{cM}/\sigma_0$ in the range of $1 \ldots 12$, respectively. It is recalled that $\sigma_{cM}/\sigma_0$ varies with temperature as discussed in Section 3.2 whereas the direct experimental determination of $\sigma_{cPM}$ is rather difficult.

Firstly, the strength of the matrix is maintained constant at $\sigma_{cM}/\sigma_0 = 4.0$ and the strength of the particle-matrix interface $\sigma_{cPM}/\sigma_0$ is varied. Corresponding macroscopic stress-strain curves are plotted in Figure 8. Again, three stages are observed: ① a micro-crack originates at the grain boundary due to high stress concentration induced by dislocation pile-up; ② the micro-
crack grows and arrives at the particle-matrix interface. Subsequently, the carbide-particle is broken or debonded, which leads to softening of the cell structure and finally the micro-crack completely propagates through the second grain.

For a low strength of the interface $\sigma_{cPM}/\sigma_0 \leq 6.0$, the particle debonds once the microcrack reaches the interface. In contrast, for a high interface strength $\sigma_{cPM}/\sigma_0 > 6.0$, the microcrack propagates straight through the particle. However, the diagram at the left-hand side of Figure 8 shows that this switch in the mechanism has no significant influence on the macroscopic stress-strain curve.

In contrast, Figure 9 shows that the strength $\sigma_{cM}$ (relative to the yield stress $\sigma_0$) of the ferritic matrix has a very strong influence on the macroscopic stress-strain behaviour. High values of $\sigma_{cM}/\sigma_0$, i.e., a higher temperature, lead to a later initiation of cleavage and thus to a more ductile behaviour. In contrast, less energy can be dissipated for low values $\sigma_{cM}/\sigma_0$, i.e. at low temperatures. For $\sigma_{cM}/\sigma_0 = 1.0$, even no crack arrest stage can be identified anymore.

Similar tendencies are observed for weak particle interfaces $\sigma_{cPM}/\sigma_0 = 0.1$ for which the
Influence of strength of matrix for weak particles $\sigma_{cPM}/\sigma_0 = 0.1$

Influence of strength of matrix for strong particles $\sigma_{cPM}/\sigma_0 = 12.0$

Particles debond, see Figure 10. This figure contains also the case of classical plasticity for which no initiation of cleavage is obtained at all in the considered range of uni-axial loading, even at a relatively low cleavage strength of the matrix $\sigma_{cM}/\sigma_0 = 2.0$.

Finally, Figure 11 illustrates the effect of the strength of the matrix for a very strong particle-matrix interface $\sigma_{cPM}/\sigma_0 = 12.0$. Microscopically, the high strength of the interface leads to a change of the mechanism from debonding to breakage of the particle. However, a comparison of the macroscopic stress-strain curves to those with an intermediate strength of the interface in Figure 9 does not indicate a significant difference.

Independent of the particular choice of the strength $\sigma_{cPM}$ of the interface, it can be concluded that much higher values of the strength $\sigma_{cM}$ of the ferritic matrix can be used with the gradient theory than with conventional theory. Such higher values are more realistic since they lie closer to the theoretical strength $\sigma_{thcM} \approx E/10$ of the material. The remaining difference between $\sigma_{cM}$ and $\sigma_{thcM}$ might be attributed to the fact that anisotropy, both of elasticity and plasticity, are not taken into account in the present model.
4.3 Distribution of dislocation densities

The relationship between dislocation densities and effective plastic strain and its gradient is given in Eq. (6). The material parameters for the ferritic matrix are chosen as in [15, 27, 28, 42-44]: Taylor’s factor $m$ is taken as $m = 2.75$ (corresponding to BCC polycrystalline metals), Burgers vector is chosen as $b = 0.248 \text{ nm}$ and the empirical coefficient amounts to $\alpha = 0.3$.

Figure 12 shows the evolution of the densities of SSDs and GNDs for the case of intermediate strengths $\sigma_{cPM}/\sigma_0 = 4.0$ and $\sigma_{cM}/\sigma_0 = 4.0$ with material length scale $\ell/R = 0.2$, whose stress-strain curve with respective markings 1-6 was shown in Figure 6. During the propagation of the micro-crack, the macroscopic stress recovers two times (stage 3 and stage 5). This behaviour is explained by the evolution of SSDs in the cell model. The SSD density increases with increasing effective plastic strain at the crack tips, which leads to enhanced strain hardening. For a weak interface, the SSD density around the crack tip is smaller compared to that of a strong interface. Therefore, the strain hardening increases gradually, in contrast to a strong interface. Vice versa, the maximum principal stress reaches the strength of the ferrite (the matrix) slower than with the strong interface. Consequently, the micro-crack mechanism is quasi-brittle for the model with the strong interface.

According to [28, 45], the GND density $\rho_G$ at grain boundaries in metallic alloys lies in the range of $10^{15} \ldots 10^{18} \text{ m}^{-2}$. Furthermore, $\rho_G$ often exceeds the SSD density $\rho_S$ by one or two orders of magnitude. Both aspects are reproduced realistically by the simulations, see Figure 12b. At elevate position on the strain hardening curve (stage 1), high values of GND density are concentrated at the grain boundary indicating a dislocation pile-up. The associated high local stresses reach the strength $\sigma_M$ of the ferritic matrix thus triggering the initiation of a micro-crack. The crack grows dynamically but arrests (stage 2). Notice that GND density still accumulates with ongoing loading. Therefore, when the crack arrives at the particle-matrix interface, both GNDs and SSDs at the crack tip contribute to the recovery of strain hardening (stage 3). Subsequently, the microcrack from the particle coalesces with the cleavage microcrack of the matrix (stage 4). The propagation of the micro-crack and the associated local stress relief cause a redistribution of GNDs at the flanks of the micro-crack. The density of SSDs at the crack tip in the second grain increases since further plastic deformations are necessary to drive the crack stably through the outer grain 2 until it cleaves completely. This event finally induces the drop in the stress-strain curve (stage 5).

5 Summary and conclusions

In the present study, an axi-symmetric cell model was employed to study qualitatively the interaction of dislocation pile-up with cleavage initiation at carbide particles and at grain boundaries in ferritic steels. The plastic behaviour of the ferritic matrix was described by a higher-order theory of plasticity which incorporates the gradient of the equivalent plastic strain. Despite its isotropic behaviour, such a theory can describe the dislocation pile-up at large-angle grain boundaries if micro-hard jump conditions are utilized there. The performed simulations show that this dislocation pile-up leads to considerably increased local stresses which trigger initiation of cleavage of the ferrite. Both, potential cleavage as well as breakage or debonding of carbide particles were modelled by a cohesive zone.

Systematic parameter studies were performed with respect to the influence of the strengths of ferrite, carbide and their interface as well as with respect to the size of the carbide relative to the intrinsic length $\ell$ of the gradient model. The parameter studies showed that the strength of
Figure 12: Evolution of dislocation densities: (a) SSDs, (b) GNDs
the carbide has an influence on the microscopic path of crack propagation, which is, however, hardly correlated to the macroscopic stress-strain behaviour. In contrast, the ratio $\sigma_{cM}/\sigma_0$ of cleavage strength of ferrite to its yield stress has a strong influence on the macroscopic ductility. This ratio is directly correlated to the temperature. Considerably higher values of the cleavage strength $\sigma_{cM} > 10\sigma_0$ could be realized in the gradient-enriched model than in models with conventional plasticity leading to more realistic micro-structural failure mechanisms. The intrinsic length of the gradient theory is related to the mean free path of dislocations. The ratio of intrinsic length to the carbide size, as well as the size of the grain the carbide is embedded in, were found to have a strong effect on the macroscopic strain hardening behaviour and on potential arrest of microcracks which were nucleated at grain boundaries. These mechanisms cannot be simulated within the conventional theory of plasticity. Thus, the gradient enhancement and the formulation of suitable jump conditions at grain boundaries are essential to micro-mechanical modelling of the ductile-brittle transition of ferritic steels.

Future quantitative studies must determine the intrinsic length $\ell$, and the penalty parameter $\hat{h}$, from suitable experiments like indentation tests for a particular steel. Furthermore, the employed axi-symmetric cell model required that the carbide be located within the ferrite grain. Future 3D simulations are needed to address carbide particles located at grain boundaries.

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References


Supplementary material

Source code of implementation of gradient plasticity in Abaqus.

Appendix: Implementation of the modified Newmark method

In the modified Newmark method, the vectors of nodal accelerations and velocity, \( \mathbf{a} \) and \( \mathbf{v} \), respectively, are integrated within one time increment \( \Delta t = t^{m+1} - t^m \) as

\[
\mathbf{v}^{m+1} = \mathbf{v}^m + \Delta t \left[ (1 - \gamma)\mathbf{a}^m + \gamma \mathbf{a}^{m+1} \right],
\]

\[
\mathbf{u}^{m+1} = \mathbf{u}^m + \Delta t \mathbf{v}^m + \frac{(\Delta t)^2}{2} \left[ (1 - 2\beta)\mathbf{g}^m + 2\beta \mathbf{a}^{m+1} \right],
\]

(cf. e. g. [46]). These equations can be solved for the updated accelerations

\[
\mathbf{a}^{m+1} = \frac{1}{\beta(\Delta t)^2} (\mathbf{u}^{m+1} - \mathbf{u}^m) - \frac{1}{\beta \Delta t} \mathbf{v}^m - \frac{1 - 2\beta}{2\beta} \mathbf{a}^m.
\]

The acceleration vector can be inserted to the discretised equations of motion \( 0 = \mathbf{M} \cdot \mathbf{a}^{m+1} + \mathbf{F}_{\text{int}}^{m+1} - \mathbf{F}_{\text{ext}}^{m+1} \) yielding \( 0 = \mathbf{F}_{\text{int}}^{m+1} - \mathbf{F}_{\text{ext}}^{m+1} \) with an equivalent vector of internal nodal forces

\[
\mathbf{F}_{\text{int}}^{m+1} = \mathbf{F}_{\text{int}}^{m+1} + \mathbf{M} \cdot \left[ \frac{1}{\beta(\Delta t)^2} (\mathbf{u}^{m+1} - \mathbf{u}^m) - \frac{1}{\beta \Delta t} \mathbf{v}^m - \frac{1 - 2\beta}{2\beta} \mathbf{a}^m \right].
\]
In order to extend a static FEM program towards dynamic problems, thus, the following steps are necessary:

1. The nodal values $v^m$ and $a^m$ of velocity and acceleration, respectively, from the last time increment need to be stored.

2. The mass matrix $M$ needs to be computed.

3. The additional contribution of the inertia terms to the nodal forces in Eq. (16) needs to be incorporated as well as the corresponding term $\frac{1}{\rho^c \Delta t^2} M$ to the stiffness matrix $\partial \tilde{F}_m^{n+1} / \partial u^{n+1}$.

These steps can first be performed individually for each element without changes to the global FEM program and secondly without knowledge of the internal nodal forces $F_{int}^{m+1}$.

We implemented the procedure in Abaqus/Standard as user-defined elements via the UEL interface. Such a user-defined element needs to be super-imposed to each thermomechanical built-in element of Abaqus. The user-defined element needs to reserve space for the nodal quantities $v^m$ and $a^m$, respectively, in form of “solution-dependent variables” (SDVs). Secondly, it computes the updated accelerations and velocities by Eqs. (13) and (15) based on the current estimate $u^{m+1}$ for the nodal displacement. Subsequently, the element mass matrix is computed which is required for the user-defined element to compute the inertia terms, i.e. the second term on the right-hand side of Eq. (16). Finally, the user-defined element returns this element contribution to the nodal forces and the respective contribution to the stiffness matrix to the global program.

This methodology can be used with any built-in element of Abaqus. It is only required that the same element topology and shape functions are used in the superimposed user-defined elements. For the present study, values $\beta = 1/2$ and $\gamma = 1$ are used for the Newmark parameters corresponding to an Euler-backward scheme.