Numerical Stability of the Cohesive Zone Approach in Simulated Initiation and Growth of Intergranular Cracks in Polycrystalline Aggregates

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ABSTRACT

Understanding and controlling early damage initiation and evolution are amongst the most important issues in nuclear power plants. Integranular cracking has been known to occur in both austenitic steels and nickel based alloys. Modelling efforts are under way to understand this phenomenon on the grain-level scale where the influence of the microstructure plays an important role. Here, the initiation and evolution of integranular cracking can be modelled using the advanced finite element approaches with explicit account of the grains, their crystallographic orientation and explicit inclusion of grain boundaries. The cohesive-zone approach, with damage initiation and evolution, can be used for grain boundaries. However, the stability of such an approach can be problematic, especially in cases where there are a number of intergranular cracks. These cracks can form complex networks which can have a negative impact on the stability of the analysis. This work addresses some of the issues related to the stability. The influence of the finite element individual model parameters like convergence controls and numerical viscosity on the model convergence is looked at. The effects are demonstrated on a simple geometry containing 3 grains. It is shown that the numerical viscosity has the highest beneficial influence on the convergence. However values of numerical viscosity of more than 10 % of the time step should be avoided.

1 INTRODUCTION

The cohesive zone approach [1, 2] can be used for modeling decohesion between interfaces. In polycrystalline aggregate models it can be used for modeling the grain boundaries and intergranular crack initiation and evolution [3, 4]. This is of particular interest for understanding early intergranular stress corrosion crack propagation. However, numerical stability issues of ten accompany such simulations, particularly in the cases where polycrystalline aggregates are
modeled and cohesive elements are used to model the complex 3D networks of grain boundaries \cite{5}. A number of model parameters can have an effect on the stability such as mesh density, numerical controls and viscosity, etc.

In this paper a systematic approach is undertaken to assess the effect that these parameters have. The finite element model is presented first with the cohesive zone constitutive response. Numerical examples demonstrate the effects of individual parameters. Recommendations and conclusions are given at the end.

2 THE FINITE ELEMENT MODEL

The finite element model is composed out of three grains, see Fig. 1. The grain boundaries are displayed on the right-hand side. They form the “Y” shape and connect the three grains. The grains are meshed using the linear tetrahedra elements (ABAQUS type C3D4), while the grain boundaries are meshed using triangular prism elements (ABAQUS type COH3D6).

The length of the model in the X direction is 4 mm. The loads are applied by moving the nodes on the right-front surface in the positive X direction by up to 0.01 mm, resulting in macroscopic specific deformation in the X direction of up to $\epsilon = 0.025$ (assuming grain boundaries have no damage). The nodes on the left-back surface are constrained in all three directions to prevent rigid body movement.

![Figure 1: Model and boundary conditions. Different colors indicate different grains. Right-hand side shows the grain boundaries.](image)

2.1 Constitutive model and material properties

Illustrative material properties are used in the presented example. Isotropic elasticity is used for grains. Young modulus of 200 000 MPa and Poisson ratio of 0.3 is used.

The grain boundaries are modeled using cohesive elements with traction-separation constitutive response \cite{6, 7}. Fig. 2 displays the constitutive response along the element’s normal (thickness) direction. Initially, the traction (stress) in the element is linearly dependent upon the separation of the element’s faces, $\delta$. As the separation increases beyond the damage initialization value, $\delta_n^0$, the damage increases, linearly decreasing the tensile load carrying capability of the element. When separation reaches the critical value, $\delta_f$, the element is no longer able to sustain the tensile load. However, it is still able to sustain a compressive load as the damage
only affects the tensile properties of the element. Area under the curve ABD can be referred to as elastic energy \( E_n^0 \) while the area under the curve BCD as fracture energy \( E_f^0 \).

Traction (stress) in the element’s normal direction, \( t(\delta) \), is defined by Eq. (1)

\[
t(\delta) = (1 - D(\delta))K_{nn} \frac{\delta}{L_{coh}^0}
\]

where \( \delta \) stands for the separation, \( D(\delta) \) damage evolution, \( K_{nn} \) cohesive’s element elastic modulus in the normal direction and \( L_{coh}^0 \) numerical thickness of the cohesive element. Damage evolution is defined by Eq. (2).

\[
D(\delta) = \begin{cases} 
\delta < \delta_n; & 0 \\
\delta \geq \delta_n; & \frac{\delta^f(\delta - \delta_n)}{\delta(\delta_n - \delta_n)} 
\end{cases}
\]

The grain boundaries are assumed to have the same elastic modulus in the normal direction as the grains themselves, \( K_{nn} = 200 \text{ MPa} \) is used for all the cohesive elements. It is assumed that the numerical thickness of the cohesive elements is \( L_{coh}^0 = 1.0 \times 10^{-3} \text{ mm} \). Furthermore, it is assumed that the damage in the cohesive elements initiates at \( \epsilon_n^0 = 0.001 \), resulting in \( \delta_n^0 = 1.0 \times 10^{-6} \text{ mm} \). \( \delta^f_n \) is taken as 200 times larger than \( \delta_n^0 \), resulting in \( \delta_n^f = 2.01 \times 10^{-4} \text{ mm} \) and \( \epsilon_n^f = 0.201 \).

### 3 THE RESULTS

A model with medium mesh density, displacement based cohesive-zone definition [7] and no artificial viscosity is taken as a initial model. The displacement-based loads are separated into two steps. In the first step the nodes on the right-front surface are moved in the positive X direction by up to 0.004 mm, resulting in macroscopic specific deformation in X direction of \( \epsilon = 0.001 \). Since this is equal to \( \epsilon_n^0 = 0.001 \), this should result in only elastic strains and no damage in the cohesive elements. In simulations, however, stress concentrations were observed at the triple points between the grains, resulting in damage being initialized already at the end of the first step, see Fig. [3] and Fig. [4].
Figure 3: Damage due to stress concentrations at the triple points between the three grains. End of step 1.

In the second step the displacements are increased up to 0.01 mm, resulting in macroscopic specific deformation in X direction of $\epsilon=0.025$—about 80 times smaller than the specific deformation at which the cohesive element fails ($\epsilon_f=0.201$). However, the simulation stopped at the end of the first step due to the convergence issues.

Figure 4: Mises stress at the end of step 1.

Identical results were obtained when switching to energy based cohesive-zone definition [7]. In this definition, the area underneath the curve ABC in Fig. 2 is defined ($E_f$) instead of providing $\delta_f$. This is according to expectation.

To improve the convergence, discontinuous convergence controls can be applied. In this case the number of iterations prior to beginning of any checks on the convergence rate are increased. However, although the increased number of iterations was in fact observed, this did not have any effect on the final results. The simulation again stopped at the end of the first step. Similarly, the 5 times increase in the time of the second step did not have any effect.

In the next step, artificial viscosity was introduced to the model. To improve the convergence viscous stiffness degradation, $D_\nu$, can be used instead of $D$. The two are related through Eq. (3).
where \( \mu \) is the viscosity parameter representing the relaxation time of the viscous system and \( D \) is the degradation variable evaluated in the inviscid backbone model, Eq. (2) [7].

\[
\dot{D}_\nu = \frac{1}{\mu} (D - D_\nu)
\]

(3)

This delays the damage and increases the stability of the simulation. For a linear time increase of the separation \( \delta_n \) one can obtain a theoretical solution of the Eq. (3), see [8]. The resulting damage is given by Eq. (4), while the traction in the cohesive element is given by Eq. (6).

\[
D_\nu(t) = \begin{cases} 
0 & \text{if } \delta(t) \leq \delta_n^0 \\
\frac{\delta_n^f}{\delta_n - \delta_n^0} - e^{\frac{\nu}{\mu} \frac{1}{t_{step}}} \delta_n^0 \ln |t| + \sum_{i=1}^{\infty} \left( \frac{t_{step}}{\mu \delta_n^0} \right)^i \frac{1}{i!} & \text{if } \delta(t) > \delta_n^0
\end{cases}
\]

(4)

\[
C = \frac{1}{\mu} \delta_n^0 \delta_n - \delta_n^0 \ln \left| \frac{t_{step} \delta_n^0}{\delta_n^0 - \delta_n^f} \right| + \sum_{i=1}^{\infty} \left( \frac{t_{step} \delta_n^0}{\mu \delta_n^0} \right)^i \frac{1}{i!} - e^{\frac{t_{step} \delta_n^0}{\mu \delta_n^0}} \frac{\delta_n^f}{\delta_n - \delta_n^0}
\]

(5)

\[
t_n(t) = \begin{cases} 
\frac{\delta_n^f}{t_{step}} \cdot t \cdot \frac{1}{T_0} & \text{if } \delta(t) \leq \delta_n^0 \\
K_n \frac{\delta_n^f}{t_{step}} \cdot t \cdot \frac{1}{T_0} & \text{if } \delta(t) > \delta_n^0
\end{cases}
\]

(6)

In the above equations the symbol \( t_{step} \) refers to the length of the time step. Note, that in a complex structure the displacements are unlikely to be linearly time-dependent. Still, the expression above can be used for assessing basic behaviour of the cohesive elements.

Fig. 5 shows the resulting impact. Four distinct effects can be observed: a) the smoothing of the traction-separation response, b) increased maximum traction, c) the delay in the damage evolution and e) the area under the curve increases with increased \( \mu \). For viscosity parameter, \( \mu \), equal to 1 % of the step time, \( t_{step} \), the increase of the maximum traction is relatively small, the smoothing of the curve and the delay in the damage evolution contribute to decreased convergence issues. For higher values of viscosity parameter one can already observe significantly increased maximum traction, while the delay in the damage evolution can result in the total damage at displacement larger than initially foreseen \( \delta_n^f \). The viscosity parameter \( \mu \) should therefore not be higher than 10 % of \( t_{step} \). Also, note that the \( t_n \) depends upon the ratio \( \delta_n^0/\delta_n^f \).

At small ratios, the maximal traction above the foreseen value \( t_n^0 \) is higher compared to the higher ratios, cf. Fig 5 top and bottom. The fraction of the elastic displacements compared to the total displacements at complete failure therefore also plays a role.

In the next step viscosity of 0.5 % of step time and 1 % of step time was introduced. This resulted in significantly improved convergence and in both cases the simulations successfully reached their planned end. The cohesive layer between the larger right-hand side grain and the smaller central grain and the layer between the two larger grains completely decoupled due to full damage of the cohesive elements in these two layers, see Fig. 6.
Figure 5: The effect of viscous regularization [8]. Top: $\delta_n^0/\delta_f^0=0.048$. Bottom: $\delta_n^0/\delta_f^0=0.071$. 
Figure 6: Mises stress at the end of step 2. Top: viscosity of 0.5% of step time used. Bottom: viscosity of 1% of step time used.
4 CONCLUSIONS

In this work a simplified model of a polycrystalline aggregate, composed of three grains is presented. A cohesive-zone approach is used to explicitly account for the grain boundaries between the grains. The influence of the finite element individual model parameters like time step length, convergence controls and numerical viscosity on the model convergence is looked at. The effects are demonstrated on a simple geometry containing 3 grains. It is shown that the numerical viscosity has the highest beneficial influence on the convergence. Numerical viscosity values of more than 10% of the time step should, however, be avoided.

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