Cohesive model application to micro-crack nucleation and growth

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Abstract

The process of micro-crack nucleation and the first stages of micro-meso-crack propagation are analyzed with the help of a cohesive, finite element model. The loaded material cell containing an inclusion is presented. The model is based on experimental observations. The inclusion–matrix interface and planes of potential crack propagation in the inclusion and matrix are modeled with the cohesive elements implemented in ABAQUS. Both element-based and surface-based approaches are used. The material constants used in the calculations are hypothetical, but based on data relevant to the real materials and reported in the literature. The influence of the cohesive element parameters (that is, peak stress and fracture energy) as well as the influence of constraint on the sequence of events during loading of the material cell are analyzed. Relations between selected parameters of the model leading to inclusion fracture or the debonding process of an inclusion are established.

1. Introduction

Fractographic observations reveal modes of void nucleation. Homogeneous, strong inclusions debond from a matrix (Fig. 1a,b). In this case, debonding starts from the opposite points lying along a loading line. The load increase leads to the total debonding of an inclusion from a matrix and to the growth of a void (Fig. 1f). The void resembles a sphere irrespective of the initial shape of the inclusion. Weaker inclusions, especially those which are a conglomerate of several smaller inclusions, are prone to break (Fig. 1c,d). In this case, fractographic images reveal that the fracture of the inclusion had been the first stage of damage to a cell and then the debonding of the inclusion from the matrix took place while a new void was growing.

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In the literature several attempts to formulate the criterion for void nucleation can be observed. Among the first was the Argon criterion (1), modified by other authors (Argon (1976), Argon and Im (1975), Argon et al. (1975)):

$$\sigma_v = X\sigma_m + Y\sigma_{eq}$$  \hspace{1cm} (1)$$

where $\sigma_m$ is the hydrostatic stress, $\sigma_{eq}$ is the Huber–Mises equivalent stress, X and Y are weight parameters and $\sigma_c$ is the critical stress.

The physical meaning of this criterion is doubtful, and determination of the critical stress is very difficult. Examples of values of critical stresses are given in Table 6 in Pineau and Pardoen (2007). As the authors point out, the table has numerous shortcomings and demonstrates how difficult the analysis of void nucleation is.

An analysis of the fracture process that takes into consideration the behavior of inclusions can be made according to different strategies. In the case of the Gurson–Needleman–Tvergaard model, void nucleation is described by statistical parameters (Chu and Needleman (1980), Kwon and Asaro (1990)). In another approach, the void nucleation is taken into account assuming the value of the initial void fraction or by direct modeling of voids (Hütter et al. (2014), Pardoen and Hutchinson (2003)).

Images present only a small neighborhood of inclusion. Modeling of the void/microcrack nucleation process in a model of a real object is hard but possible work as shown by attempts in papers Huber et al. (2005) and Hütter et al. (2014). However, using a representative elementary volume could be more efficient. The size of the cell can be determined after analysis of the material microstructure. In such a case it is possible to achieve results with a low computations cost.

The void nucleation stage begins from the fracture of an inclusion or the debonding of an inclusion from a matrix. Which of these processes is active depends on many factors. In the paper Babout et al. (2004) it was shown that in soft matrix the stress does not grow beyond a critical level and debonding of the inclusion from the matrix takes place. A hard matrix favors the inclusion fracture. In papers Dighe et al. (2002) and Lewandowski et al. (1989) the influence of the inclusion size on fracture of the inclusion was analyzed. An important factor for the void nucleation process is also the shape of the inclusion (Neimitz and Janus (2016b)) and their distribution (Kwon and Asaro (1990)).

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In a number of papers the tool for analysis of the state of stress and the behavior of inclusions during the fracture process is the Gurson model. However, the cohesive model based on fundamental works by Barenblatt (1959) and Dugdale (1960) can also be used. The most important parameters in this model are the cohesive stress and work of separation (Pineau and Pardoen (2007)). The shape of the traction–separation curve depends on the type of fracture mechanism modeled and is not very important (Tvergaard and Hutchinson (1992)).

Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>E</td>
<td>Young's modulus</td>
</tr>
<tr>
<td>$G_{IC}, G_{IE}$</td>
<td>critical strain energy release rates for Mode I and for Mode II</td>
</tr>
<tr>
<td>$G_{TIC}$</td>
<td>critical strain energy release rate</td>
</tr>
<tr>
<td>$T$</td>
<td>the stress in the second term of the Williams solution</td>
</tr>
<tr>
<td>$u_1, u_2$</td>
<td>displacement vector components</td>
</tr>
<tr>
<td>$f^*$</td>
<td>work of separation (cohesive energy)</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Poisson's ratio</td>
</tr>
<tr>
<td>$\sigma_{cr}$</td>
<td>critical stress</td>
</tr>
<tr>
<td>$\sigma_{eq}$</td>
<td>the Huber–Mises equivalent stress</td>
</tr>
<tr>
<td>$\sigma_m$</td>
<td>mean stress</td>
</tr>
<tr>
<td>$\sigma_{max}$</td>
<td>maximum value of cohesive stress (peak or cohesive stress)</td>
</tr>
<tr>
<td>$\sigma_0$</td>
<td>yield stress</td>
</tr>
<tr>
<td>$\sigma_{n,max}$, $\tau_{s,max}$</td>
<td>maximum value of cohesive stress for Mode I and for Mode II</td>
</tr>
</tbody>
</table>

2. Materials used in model

In the papers Faleskog et al. (1998) and Gao et al. (1998) 21/4Cr1Mo steel was investigated. The main inclusions in this material are manganese sulfides. The size of the inclusions ranges from 1 μm to 5 μm and the average distance between them is approximately 100 μm. The Young's modulus (E) is 206 GPa, yield strength ($\sigma_0$) is 210 MPa and hardening exponent (n) is equal to 5. The critical value of the J-integral can be evaluated using the $J_R$-curve and it is equal to 350 kJ/m². This steel is used as the matrix material in a model of the material cell. The inclusion is composed of MnS. Since the inclusion is considered as linear elastic, the only material parameters important for the model are the Young's modulus and Poisson's ratio ($\nu$). In the PhD thesis by Juvonen (2004), the Young's modulus of manganese sulfides was determined in the range 68–138 GPa and Poisson's ratio was 0.3; thus, a value of 100 GPa for the Young's modulus is assumed in the computer simulations.

![Image](Image 217x171 to 298x256)

Fig. 2. (a) Material cell; (b) boundary conditions; (c) cohesive zones.

3. The model geometry

The plane strain is assumed, therefore the inclusion takes the shape of a cylinder of infinite length (McClintock (1968)). Based on material microstructure observations, the size of the material cell in the two other directions was assumed to be equal to 100 μm and the diameter of the inclusion 5 μm. Due to the symmetry, only 1/4th of the cell is modeled (shaded area in Fig. 2a).
4. Boundary conditions

The material cell is virtually located in the vicinity of the crack tip. In many works the influence of in-plane and out-of-plane constraint on material fracture is highlighted (Betegon and Hancock (1991), Larsson and Carlsson (1973), Neimitz and Dzioba (2015), Neimitz and Galkiewicz (2006)). In order to keep a high level of constraints specific for the geometries with long cracks, the displacements are applied to the elementary cell according to Fig. 2b. In paper Galkiewicz (2015) the relation between the displacement ratio \( u_1/u_2 \) and the level of in-plane constraint for the analyzed material is established in the form (2):

\[
\frac{u_1}{u_2} = (0.214*\frac{T}{\sigma_0}) - 0.169
\]

where: \( T \) is the stress in the second term of the Williams solution (Al-Ani and Hancock (1991)).

Based on the experimental observations, it is assumed that the maximum value of displacement \( u_2 \) at which the material cell is damaged is 2 \( \mu \)m, i.e. 4\% of the material cell height. The value of displacement \( u_1 \) for constraint level \( T=0 \) is -0.169 \( \mu \)m.

5. The numerical model

In the numerical model the 4-node, bilinear plane strain elements (CPE4I) are used. There are three cohesive zones (see Fig. 2c) in the model. In zone A the interaction between the inclusion and matrix is modeled using a surface-based approach. It is assumed that in this region mixed-mode fracture is possible. Zones B and C are located in the plane of the potential cracking of the inclusion and matrix. Both regions are modeled using an element-based approach. Due to the symmetry, the nodes in zones B and C are subjected to additional constraints. The nodes in these zones are shrunk, so the initial height of the cohesive zones is equal to zero. Additionally, to avoid uncontrolled movements of nodes located in the symmetry plane, their displacements are tied with displacements of corresponding nodes connected with the matrix.

6. Behavior of the cohesive zones

The most important properties of the bilinear cohesive element applied in ABAQUS are shown in Fig. 3a. To describe the behavior of the cohesive zone, the cohesive stress and energy of separation for two modes of loading should be defined. For simplicity, it is assumed that the peak stress and the cohesive energy are equal for each mode of loading within each zone (in zones B and C only mode I is assumed).

To inspect how the peak stress for mode II influences the results of simulations, several computations were carried out, with values of peak stress for mode II in zone A changing in the range from 0.3 to 1.5 of the peak stress for mode I. The results show that the cohesive stress for mode II in zone A does not influence the process of cell damage.

In zones B and C the symmetry of the problem requires that the stiffness of the elements in the cohesive zones must be two times greater than the stiffness of adjacent material. Thus, the cohesive energy is also two times reduced (Fig. 3b).
It is assumed that in zone A mixed-mode fracture is possible. In this case, the damage initiation criterion has the form (3):

$$\left(\frac{\sigma_n}{\sigma_{n,\text{max}}}\right)^2 + \left(\frac{\tau_s}{\tau_{s,\text{max}}}\right)^2 = 1$$

(3)

where $\sigma_{n,\text{max}}$ is the peak stress for mode I and $\tau_{s,\text{max}}$ is the peak stress for mode II. In order to limit the number of variables, it is assumed that $\sigma_{n,\text{max}} = \tau_{s,\text{max}}$.

In the softening stage, the energy-based damage evolution is assumed according to the Benzeggagh–Kenane relation (Abaqus (2012), Benzeggagh and Kenane (1996)) (4):

$$G_{TC} = G_{IC} + (G_{IIC} - G_{IC}) \left(\frac{G_{II}}{G_{I} + G_{II}}\right)^{\eta}$$

(4)

where: $G_{TC}$ is the critical strain energy release rate, $G_{IC}$ and $G_{IIC}$ are the critical strain energy release rates for mode I and mode II and $\eta=2.284$.

The tests proved that the changes of $G_{IIC}$ in the range 0.7–1.3$G_{IC}$ do not affect the results.

7. The cohesive zones properties

The value of critical stress for MnS in Hardox-400 steel was estimated in the paper Neimitz and Janus (2016a) as 1400 MPa, whereas Beremin proposed 1100 MPa but for A508 steel (Beremin (1981)). The difference arises from the different properties of steels. The yield stress of Hardox-400 ($\sigma_0=1000$ MPa) is more than two times higher than the yield stress of A508 steel ($\sigma_0=450$ MPa). Since the mechanical properties of A508 steel are closer to the material investigated in this paper, the value of 1100 MPa for the peak stress of the inclusion was adopted.

Beremin proposed also the critical stress value of 800 MPa for debonding of the MnS inclusion from the matrix. This value was used in the model.

In earlier studies (Galkiewicz (2015) and Gao et al. (1998)) on 21/4Cr2Mo steel, the peak stress in the cohesive zone was established at the level 1470 MPa (seven times the yield stress) for high constraint.

To estimate the work of fracture of the MnS and matrix, fractographic observations in Neimitz and Janus (2016a) were used. On this basis it was assumed that MnS particles fracture at an overall strain level of 1% approximately if the inclusion is not homogeneous. The matrix can be totally damaged at an overall strain of 4% provided the constraint level is high. To obtain such a result during simulations, the cohesive energy of the inclusion is assumed to be 240 J/m².

The results of papers Neimitz (2008) and Siegmund and Brocks (2000) prove that the work of separation strongly depends on the specimen geometry and constitutes only a small part of the total energy of fracture (even less than 1%). Therefore the cohesive energy of the matrix is assumed to be equal 2400 J/m² i.e. 10 times more than for the inclusion. At such level of work of separation, the elementary cell is totally damaged at an overall strain level of 4% approximately.

8. Analysis of inclusion behavior for identical fracture properties of zones A and B

The aim of the analysis in this section is to establish the relations between the properties of the cohesive zones leading to the inclusion cracking with simultaneous partial debonding of the inclusion from the matrix (Fig. 1c,d). To reduce the extensive number of parameters, it is assumed that the properties of zone C are constant in each simulation. In the first step of analysis, the properties of zones A and B are the same. The value of the separation work in zones A and B is assumed to be equal to 10% of the fracture work of zone C, and the cohesive stress value for zones A and B is equal to 75% of cohesive stress for zone C. The cohesive properties used in the simulation are listed in Table 1.
As a result of the simulation the surface on the material cell after cracking in the vicinity of the inclusion is presented in Fig. 4a. A new surface is created and no debonding of the inclusion from the matrix is noticed.

Fig. 4. (a) Result of 1st simulation; (b) Result of 2nd simulation; (c) Result of 3rd simulation; Result of 4th simulation.

9. Simulation of debonding of the inclusion from the matrix

In order to obtain detachment of the MnS particle from the matrix, the peak stress in zone A was reduced. The reduction was done in such a way that the critical displacement at which the interaction between the inclusion and the matrix vanishes is kept unchanged. This requires a reduction of the cohesive energy (see Fig. 3c).

The reduction of cohesive stress in zone A below the level of 0.69σ_{max} of the matrix material causes debonding of the inclusion from the matrix without the inclusion cracking (Fig. 1f). The debonding starts at the points where the vertical axis of the cell intersects the edge of the inclusion. The total detachment of the inclusion from the matrix is followed by fracture of the matrix material. The cohesive properties used in the second simulation are listed in Table 2. It turns out that the change in constraint caused by debonding of the inclusion from the matrix results in partial breaking of the matrix material (Fig. 4b). That confirms the dependence of the cohesive zone parameters on the constraint level.

10. Simulation of inclusion fracture with simultaneous debonding of the inclusion from the matrix

The parameters assumed in Table 2 do not lead to damage of the inclusion. So, the peak stresses for zones A and B were reduced to the value 800 MPa, suggested by Beremin as the cohesive stress for the inclusion–matrix interface. The new set of parameters (Table 3) leads to cracking of the inclusion with simultaneous debonding of the inclusion from the matrix (Fig. 4c). At the end of the loading process the elementary cell again is not damaged totally.

Further reduction of the peak stress in zones A and B accelerates the detachment process of the inclusion from the matrix. Exemplary results for the cohesive parameters given in Table 4 are presented in Fig. 4d.
If the maximum stresses in zones A and B are lower than \(0.25\sigma_{\text{max}}\) for zone C, the active mechanism of cell damage again becomes the debonding of the inclusion from the matrix, but in this case the process starts in the vicinity of the horizontal axis of the elementary cell and the process is so fast that, after initiation, it takes place almost at the same moment along the whole inclusion–matrix interface.

Despite such a "weak" cohesive connection between the inclusion and matrix, it is still possible to observe simultaneous cracking of the inclusion and debonding from the matrix. The condition that must be satisfied in this case is that \(\sigma_{\text{max}}\) for zone B is smaller than \(\sigma_{\text{max}}\) for zone A. The results of simulation for the set of parameters in Table 5 are similar to Fig. 4d.

### Table 5. Properties of cohesive zones for 5th simulation

<table>
<thead>
<tr>
<th>Zone</th>
<th>(\sigma_{\text{max}}) [MPa]</th>
<th>(\Gamma) [J/m²]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zone A</td>
<td>0.24*1470=353</td>
<td>0.0321*2400=77</td>
</tr>
<tr>
<td>Zone B</td>
<td>0.23*1470=338</td>
<td>0.0321*2400=74</td>
</tr>
<tr>
<td>Zone C</td>
<td>1470</td>
<td>2400</td>
</tr>
</tbody>
</table>

### 11. Conclusions

Based on the results of behavior analysis of an inclusion of a fixed shape and size, some conclusions can be drawn:

- the main factor that determines the means of void nucleation is the relation between the peak stresses in zones A and B. In the case of a high level of cohesive stress in zones A and B (\(\sigma_{\text{max}}\) higher than \(0.69\sigma_{\text{max}}\) for zone C), the elementary cell breaks along the horizontal axis. The only protrusion on the fractured surface is caused by the difference in stiffness of the inclusion and matrix;
- lower values of cohesive stress at the inclusion–matrix interface in relation to the cohesive stress for the inclusion lead to debonding of the inclusion surface from the matrix and then damage to the matrix. The critical stresses proposed by Beremin and used in the model (800 MPa for interface and 1100 MPa for inclusion) result in separation of the inclusion from the matrix (see Fig. 5a in Beremin (1981)). The simulations prove that a peak stress in zone A smaller by 5–7% than the peak stress at zone B is sufficient to activate the process of detachment of the inclusion from the matrix;
- assuming that the strength of the cohesive bond on the inclusion–matrix interface is the same as the cohesive strength of the inclusion leads to the situation that damage of the elementary cell starts by breaking of the inclusion with simultaneous debonding of the inclusion from the matrix. This is possible only if the peak stresses for zones A and B are significantly smaller than \(\sigma_{\text{max}}\) for zone C. The cohesive stress level for zones A and B within the range 365–925 MPa i.e. 0.25–0.63 of the cohesive stress of the matrix, leads to simultaneous cracking of the inclusion and debonding of the inclusion from the matrix. So, the level of critical stress in zones A and B proposed by Beremin as the cohesive stress for the inclusion–matrix interface (800 MPa) leads to inclusion damage and simultaneous debonding of about 1/3rd of the inclusion surface from the matrix;
- a peak stress lower than 365 MPa promotes debonding of the inclusion from the matrix. However, at such a low strength of bonding between the inclusion and matrix, sulfide damage takes place, but the cohesive stress for the inclusion material should be smaller by at least 5% than the cohesive stress of the inclusion–matrix interface.

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