The Influence of the Grain Boundary Strength on the Macroscopic Properties of a Polycrystalline Aggregate

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ABSTRACT

In this work a model, based on a X-ray diffraction contrast tomography data of a stainless steel wire with a diameter of 0.4 mm is presented. 3D topology and crystallographic orientation of individual grains are directly transferred into a finite element model. The influence of the grain boundary strength on the macroscopic properties of a polycrystalline aggregate is then explored. The grain boundaries are modelled using the cohesive zone approach. Anisotropic elasticity and crystal plasticity constitutive laws are used for the bulk grain material. The macroscopic response is computed using volume averaging.

1 INTRODUCTION

The cohesive zone approach 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. This is of particular interest for understanding early intergranular stress corrosion cracking propagation. However, calibration of the cohesive element properties when applied to the grain boundaries can be tedious due to the difficulties of measuring the grain boundary properties and numerical convergence issues. Moreover, even for the macroscopic size models there are different recommendations for some of the basic properties like maximum traction and grain boundary stiffness. We can find maximum traction recommendations to be between 2.5 and 3 times the yield stress or even 50, see [1, 2, 3].

In this paper we take a top down approach to the estimation of the maximum traction of the cohesive elements used to model the grain boundaries of a polycrystalline aggregate. We simulate a numerical tensile tests. Since in the tensile tests no grain boundary damage is expected, we vary the grain boundary stiffness and strength to obtain values at which little or no grain
boundary damage occurs. These values could then be taken for grain boundaries not suscepti-
ble to intergranular stress corrosion when modeling such phenomena. The finite element model
is based on the as measured grain geometry and crystallographic orientations of a 400 µm di-
ameter stainless steel wire. The experimental data is obtained using X-ray diffraction contrast
tomography (DCT) [4, 5].

2 EXPERIMENTAL DATA

The experimental data used in this work is a DCT spatial characterization of a 0.4 µm di-
ameter wire of AISI 302 stainless steel [6, 5]. The data comprises of 362 grains and some 1600
grain boundaries. The data provides information on the crystallographic orientation in points of
a 346 by 346 by 282 grid. The experimental data can be represented as an array of 282 slices,
separated in the axial (Z) direction by 1.4 µm. For each slice, crystallographic orientation has
been measured on a 346 by 346 grid with 1.4 µm distance between the points on a grid (in the
X and Y direction). Voxels having the same crystallographic orientation constitute a grain.

3 THE FINITE ELEMENT MODEL

The framework for building a FE model is described in detail in [7]. A short description of
the most important steps is provided here.

The basic step consist of initial checks and treatment of holes in the data (typical artifacts
due to the limited number of projections available for each grain and the presence of erroneous
contrast [4, 5]). This is followed by reconstruction of grain surfaces to a user defined level of
detail using a commercial software package Amira [8]. SurfaceGen tool with unconstrained
smoothing option is used [9]. This is followed by a conversion of individual grain geometries
from a surface based definition into a 3D solid definition. Next, a FE model is created. Material
properties are assigned to individual grains, boundary conditions are defined and a FE mesh is
created. Conformal mesh between the adjacent grains is created by meshing the grain surfaces
first, followed by meshing of the grain interior. During the volume meshing operation the mesh
on the surface between the adjacent grains is preserved thus creating a conformal mesh.

The resulting FE model is presented in Fig. 1 and contains 903 109 finite elements. Fig. 2
displays the grain boundaries. These are classified into resistant (low energy) and susceptible
(high energy) grain boundaries, depending upon the crystallographic orientation of the neigh-
boring grains. In this work a simplification is used where resistant grain boundaries are defined
as coincidence site lattice (Σ3 through Σ29) grain boundaries and low angle grain boundaries
with misorientation angle between the neighboring grains below 15° following [10]. All other
grain boundaries are defined as susceptible grain boundaries.

3.1 Constitutive models

Anisotropic elasticity and crystal plasticity constitutive laws as described in [11] are used for
the bulk grains while the traction-separation cohesive law is used for the grain boundaries. For
simplification, the same material properties are applied to all grain boundaries use the material
properties.
3.2 Material properties

For bulk grains elastic constants for a single crystal AISI 304 stainless steel are used [12]: $C_{iii}=204\ 600\ MPa$, $C_{ijij}=137\ 700\ MPa$, $C_{ijij}=126\ 200\ MPa$. The crystal plasticity parameters were taken from literature [7] where they were obtained by fitting the computed macroscopic response of a polycrystal aggregate to a measured tensile test of a polycrystal sample: $h_0=75\ MPa$, $\tau_0=75\ MPa$, $\tau_0=150\ MPa$, $h_s=30\ MPa$. Crystal plasticity was implemented as a user-subroutine [13] into the finite element code ABAQUS and includes versions for small deformation theory and rigorous theory of finite-strain and finite-rotation. The latter was used in this work.

For simplification, the same material properties are applied to all grain boundaries. Constitutive thickness of the cohesive elements is taken as $T_0=1.0E-3\ mm$. All grain boundaries are modeled with damage initiation and evolution. Specific deformation at damage initialization point is taken as $\epsilon_0^n=\delta_0^n=0.001$, resulting in separation at damage initiation point $\delta_0^n=1.0E-6\ mm$. Beyond the damage initialization point the cohesive element is assumed to withstand additional separation of $\delta_0^d=200\delta_0^n=2.0E-4\ mm$ before failing completely in the tensile direction. The compressive properties are not affected by the damage. To exclude damage initiation in the two shear directions high values of $\delta_0^s$ and $\delta_0^t$ are used: $\delta_0^s=\delta_0^t=200\ mm$. A viscous damping of 0.01 has been applied to the damage function to improve the convergence during the cohesive elements damage evolution.

Basic grain boundary stiffnesses are taken as: $K_{nn}=204\ 600\ MPa$ and $K_{ss} = K_{tt} = E/[2(1+\nu)]=78\ 692.3\ MPa$. Different models are created by scaling the basic stiffnesses by factors of 0.75 to 3.5 and keeping the specific deformation at damage initiation point constant at $\epsilon_0^n=0.001$. This results in grain boundary strength (maximal stress that a grain boundary can withstand) between 0.75·204.6 to 3.5·204.6 MPa, where for simplification 204.6 is taken as a 0.2 % offset yield stress, although literature states that 0.2 % offset yield stress for AISI 304 stainless steel is 205 MPa [14]. Table 1 lists all the cases while the Fig. 3 demonstrates the principle used in varying the cohesive element properties.
Figure 2: Grain boundaries in the FE model: ■ susceptible and resistant: ■ low angle and □ coincidence site lattice Σ3 through Σ29 grain boundaries.

Table 1: Analyzed cases. Grain boundary stiffness: $K_{nn}$, $K_{ss}$, $K_{tt}$. Grain boundary strength: $t_0^o$.

<table>
<thead>
<tr>
<th>Case=Scaling factor</th>
<th>$K_{nn}$ [MPa]</th>
<th>$K_{ss}$ = $K_{tt}$ [MPa]</th>
<th>$t_0^o$ [MPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.75</td>
<td>153 450</td>
<td>59 019.2</td>
<td>153.45</td>
</tr>
<tr>
<td>1.0</td>
<td>204 600</td>
<td>78 692.3</td>
<td>204.6</td>
</tr>
<tr>
<td>1.5</td>
<td>306 900</td>
<td>118 038.5</td>
<td>306.9</td>
</tr>
<tr>
<td>2.0</td>
<td>409 200</td>
<td>157 384.6</td>
<td>409.2</td>
</tr>
<tr>
<td>2.5</td>
<td>639 375</td>
<td>196 730.8</td>
<td>511.5</td>
</tr>
<tr>
<td>3.0</td>
<td>613 800</td>
<td>236 076.9</td>
<td>613.8</td>
</tr>
<tr>
<td>3.5</td>
<td>716 100</td>
<td>275 423.1</td>
<td>716.1</td>
</tr>
</tbody>
</table>

3.3 Boundary conditions

For all the FE models the nodes on the back surface were constrained in all three directions. Tensile displacements on the model’s front surface are applied in the axial direction up to $\epsilon=0.035$ at a strain rate of $\dot{\epsilon}=1E-6$ s$^{-1}$.

3.4 Macroscopic equivalent values

Macroscopic equivalent stress $<\sigma_{eq}>$ and macroscopic equivalent strain $<\epsilon_{eq}>$ are calculated using volume averaging, Eq. (1), with equivalent stress $\sigma_{eq}$ and strain $\epsilon_{eq}$ defined with Eq. (2) and Eq. (3).

\[
<\sigma_{eq}> = \frac{1}{V} \int_V \sigma_{eq} dV, \quad <\epsilon_{eq}> = \frac{1}{V} \int_V \epsilon_{eq} dV
\]  

\[
\sigma_{eq} = \sqrt{\frac{1}{2} \left[ (\sigma_x - \sigma_y)^2 + (\sigma_y - \sigma_z)^2 + (\sigma_z - \sigma_x)^2 + 6\tau_{xy}^2 + 6\tau_{yz}^2 + 6\tau_{zx}^2 \right]}
\]  

\[
\epsilon_{eq} = \sqrt{\frac{2}{3} \left[ (\epsilon_x - \epsilon_y)^2 + (\epsilon_y - \epsilon_z)^2 + (\epsilon_z - \epsilon_x)^2 + 6\epsilon_{xy}^2 + 6\epsilon_{yz}^2 + 6\epsilon_{zx}^2 \right]}
\]
4 RESULTS

Fig. 4 displays the computed numerical tensile tests for different grain boundary stiffnesses (and strengths). One can see that scaling does not change the tensile test curve. This is in line with expectations since the volume of the cohesive elements is practically zero and does not contribute to the volume averaging. At smaller grain boundary stiffnesses/strengths the simulations finished prematurely. This was due to numerical convergence issues. Smaller grain boundary stiffnesses result in smaller strengths, leading to the earlier damage evolution which also develops at more grain boundaries. Once the damage initializes in the cohesive elements, the literature suggests that the size of cohesive elements begins to play a role. A process zone (often called also a cohesive zone) develops in front of the crack. To be able to capture the crack evolution properly, the cohesive elements should be smaller than the process zone [15]. For a constant failure stress the process zone length is given by Eq. (4, left) [16]. On the other hand, when the failure stress varies linearly within the cohesive zone, the process zone length is given by Eq. (4, right) [17].

\[
\alpha = \frac{\pi}{8} \left( \frac{K_I}{t_0 n} \right)^2, \quad \alpha = \frac{9\pi}{32} \left( \frac{K_I}{t_0 n} \right)^2
\]

(4)

If we use \(K_{Ic}=50\) MPa m\(^{1.5}\) and \(t_0 n=205\) MPa, Eq. (4, left) results in a requirement that the cohesive element size is smaller than \(\alpha=2.3E-2\) \(\mu\)m. This is two orders of magnitude smaller than our model and is clearly beyond our current computational capacity. With a conformal mesh between the grains and the grain boundaries, such a model would result in prohibitively large number of finite elements (current model already contains 903 109 finite elements). A denser mesh of the cohesive layer compared to the surrounding bulk grain mesh would need to be created, although this might result in the stress irregularities on the interface between the non-conformal meshes. The model will have to be further developed to allow for non-conformal meshes.

With grain boundary stiffness (\(K_{nn}\)) exceeding that of the bulk material, the numerical convergence improved significantly. This is in line with the recommendations in the literature that the grain boundary stiffness should be higher than the Young modulus of the surrounding material. The reason for improved convergence is in our case the lower amount of grain boundary damage due to higher grain boundary strengths. Fig. 6 shows the percentage of the grain...
boundary area, where cohesive elements have damage above 10% and 90%. At scaling factors of 0.75 and 1.0 damage accumulates rapidly, decreasing the numerical convergence and finally leading to premature end of simulations. At scaling factor 0.75 the area of grain boundaries with high percentage of damage is relatively small, however, the damaged area is still the largest of all cases. One can observe that there is a sharp decrease of the percentage of damaged areas when increasing the grain boundary stiffness from 1.0 to 1.5$K_{nn}$, but beyond this the percentage of damaged area remains approximately the same. This suggests that a scaling of 1.5$K_{nn}$ can be used to obtain low amount of damaged grain boundaries, however, better convergence was obtained with higher scaling factors. In the conducted analyses the area under the triangle (fracture toughness) in Fig. 3 varied. The assessment of various parameters on the stability of simulations at constant fracture toughness is currently under way. Various recommendations as to the ratio $\delta_0/\delta_n$ exist [13]. Initial result indicate that reducing the $\delta_n$ has a negative impact.
5 CONCLUSIONS

A parametric study on the effects of the grain boundary stiffness and strength on the macroscopic response of a polycrystalline aggregate is presented. Measured grain geometry and crystallographic orientations of a 400 µm diameter stainless steel wire, obtained by X-ray diffraction contrast tomography [4, 5], is used. The grain boundaries are modeled using the cohesive zone approach while anisotropic elasticity and crystal plasticity constitutive laws are used for the bulk grain material. The macroscopic response is computed using volume averaging. Properties of cohesive elements that result in low amount of damage at tensile test conditions are studied, as low amount of grain boundary damage is expected under such conditions. These properties could then be taken for grain boundaries not susceptible to intergranular stress corrosion when modeling such phenomena. The finite element model is based on the as measured grain geometry and crystallographic orientations of a 400 µm diameter stainless steel wire. The experimental data is obtained using X-ray diffraction contrast tomography (DCT) [4, 5].

The results show that the cohesive elements should have higher stiffness compared to the bulk grain material. Scaling factor larger than 1.5 is sufficient to assure a low amount of grain boundary damage, however, better convergence is obtained with scaling factors of 3.0 and 3.5. Above the scaling factor of 1.5, little difference in the area of the damaged grain boundaries is observed.

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REFERENCES


