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Cohesive element approach to grain level modelling of intergranular cracking

Igor Simonovski [a,*], Leon Cizelj [b]

[a] European Commission, Joint Research Centre, Institute for Energy and Transport, P.O. Box 2, NL-1755 ZG Petten, The Netherlands
[b] Jožef Stefan Institute, Reactor Engineering Division, Jamova cesta 39, SI-1000 Ljubljana, Slovenia

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ABSTRACT

A cohesive element approach to modelling the intergranular cracking on the grain level is presented. The cohesive elements with zero physical thickness are directly inserted between the adjacent grains. These are obtained using 3D Voronoi tessellation. The grain boundary with the highest normal stress has on average 50% higher normal stress compared to the applied external load, which in this work is equal to half yield stress. Setting the maximum traction of a cohesive element equal to yield stress therefore results in limited grain boundary damage. Most of the early damage initiates at intersections of grain boundaries with the external surfaces of the model. A smaller fraction of damage develops inside the model, mostly at the triple lines where several grain boundaries come together.

A novelty in this work is the developed analytical expression for assessing the cohesive element response when using viscous regularization for alleviating the convergence issues. It shows that the viscous regularization should not be higher than 10% of the step time. Otherwise the delay in the damage evolution and the area underneath the traction-separation response of a cohesive element increase considerably. This is also demonstrated on a model with 500 grains where the time-evolution of the displacements in the cohesive elements is significantly more complicated compared to the linear assumption in the theoretical expression. Also, the fraction of the elastic displacements compared to the total displacements at complete failure plays a role, with a higher elastic part resulting in smaller increase of the maximum traction in the cohesive element.

1. Introduction

Intergranular cracking significantly depends upon the grains and grain boundaries as their properties effect both the initiation and the evolution phase. The 3D geometry of the grains also plays a significant role as it defines the resulting grain boundary network. From the modelling perspective both appropriate constitutive laws and the inherent 3D geometry of the polycrystalline aggregate need to be considered when modelling intergranular cracking at the grain level. The cohesive element approach can be used to account explicitly for the grain boundaries and has been used in a number of cases in the literature [1–3], in most cases using 2D grain structures. The transition to 3D structures is impeded by significant increase in the geometry complexity and computational time. However, this step is necessary to overcome the limitations of 2D grain structure models.

In this work a 3D finite element model of a polycrystalline aggregate with explicit account for grain boundaries is presented. Crystal plasticity is used for the grains while cohesive elements with zero physical thickness are used for grain

* Corresponding author. Tel.: +31 224 565072.
E-mail addresses: Igor.Simonovski@ec.europa.eu (I. Simonovski), Leon.Cizelj@ijs.si (L. Cizelj).

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List of symbols

C	constant
C_{ijkl}	stiffness tensor
D	damage
D_v	viscous stiffness degradation
E	young modulus
E^{coh}	cohesive energy
E_n^0	elastic energy
E^{pl}	fracture energy
h_0	initial hardening modulus
h_s	hardening modulus within stage I hardening
K_{nn}	stiffness in normal direction
K_{ss}	stiffness in first shear direction
K_{tt}	stiffness in second shear direction
t	time
t_n	traction in normal direction
t_s	traction in first shear direction
t_{step}	step time
t_t	traction in second shear direction
T_0	constitutive thickness of cohesive element
γ_{GB}	grain boundary energy
γ_S	surface energy
δ	separation
δ_n	separation in normal direction
δ_n^0	separation in normal direction at damage initialization point
δ_n^f	separation in normal direction at rupture
δ_s	separation in first shear direction
δ_t	separation in second shear direction
ϵ_n	specific deformation in normal direction
ϵ_n^0	specific deformation in normal direction at damage initialization point
ϵ_s	specific deformation in first shear direction
ϵ_t	specific deformation in second shear direction
μ	viscous regularization
ν	Poisson ratio
τ_s	reference stress
τ_0	critical shear stress

boundaries. Initiation and evolution of the intergranular cracking is then demonstrated for a large polycrystalline aggregate, with the fracture energies taken as a first step in calibration of the cohesive elements. Statistical analysis is also undertaken to estimate the effects of variation of some of the parameters. Viscous regularization is applied to improve the convergence and its effects are discussed both in terms of theory and numerical examples.

2. The finite element model

A polycrystalline aggregate is modelled using 3D Voronoi tessellation with Wigner–Seitz cells [4], see Fig. 1. It contains 500 grains and 3130 grain boundaries. A conformal mesh is created between the grains and grain boundaries. Details of the meshing procedure have been previously reported [3]. 1,200,443 linear tetrahedron elements (ABAQUS type C3D4) are used for meshing grains while 148,664 linear triangular prism elements (ABAQUS type COH3D6) are used for meshing the grain boundaries. These are classified into resistant (low energy) and susceptible (high energy) grain boundaries, depending upon the crystallographic orientation of the neighbouring grains. In this work a simplification is used where resistant grain boundaries are defined as coincidence site lattice ($\Sigma 3$ through $\Sigma 29$) grain boundaries and low angle grain boundaries with misorientation angle between the neighbouring grains below 15° following [5]. Σ value is computed as the ratio enclosed by a unit cell of the coincidence sites and the standard unit cell [6] from the Rodrigues vectors of the two neighbouring grains. Brandon [7] criterion for a proximity to a coincidence site lattice structure with proportionality constant of 10° is used. All other grain boundaries are defined as susceptible grain boundaries. The crystallographic orientations of grains are randomly distributed [8].

2.1. Loads and boundary conditions

A traction of up to 102.5 MPa, equal to half 0.2% offset yield stress of AISI 304 [9], is applied to the top surface at a rate of 0.8 MPa/s. Nodes on the bottom surface are constrained in the Y direction, nodes on the bottom, right edge (min (Y) and max