A two-scale three-dimensional boundary element framework for degradation and failure in polycrystalline materials

I. Benedetti[1,a], M.H. Aliabadi[2,b]

[1]Dipartimento di Ingegneria Civile, Ambientale, Aerospaziale e dei materiali, Università degli Studi di Palermo, Viale delle Scienze, Edificio 8, 90128, Palermo, Italy

[2]Department of Aeronautics, Imperial College London, South Kensington Campus,SW7 2AZ, London, UK.

[a]ivano.benedetti@unipa.it, [b]m.h.aliabadi@imperial.ac.uk

Keywords: Polycrystalline materials; Multiscale modelling; Micromechanics; Non-linear boundary element method.

Abstract. A fully three-dimensional two-scale boundary element approach to degradation and failure in polycrystalline materials is proposed. The formulation involves the engineering component level (macro-scale) and the material grain scale (micro-scale). The damage-induced local softening at the macroscale is modelled employing an *initial stress approach*. The microscopic degradation processes are explicitly modelled by associating Representative Volume Elements (RVEs) to relevant points of the macro continuum and employing a three-dimensional grain-boundary formulation to simulate *intergranular* degradation and failure in the microstructural Voronoi-type morphology through cohesive-frictional contact laws. The scales coupling is achieved *downscaling* macro-strains as periodic boundary conditions for the RVE, while overall macro-stresses are obtained via volume averages of the micro-stress field. The comparison between effective macro-stresses for the damaged and undamaged RVE allows to define a macroscopic measure of material degradation. Some attention is devoted to avoiding pathological damage localization at the macro-scale. The multiscale processing algorithm is described and some preliminary results are illustrated.

Introduction

Understanding materials degradation and failure is relevant for several modern structural applications. Damage and fracture can be considered at different length scales: it is widely recognized that the macroscopic material properties depend on the material microstructure[1].

Polycrystalline materials, either metals, alloys or ceramics, are commonly employed in Engineering. The microstructure is determined by the grains morphology, size distribution, anisotropy and crystallographic orientation, stiffness and toughness mismatch and by the physical and chemical properties of the intergranular interfaces. These aspects have a direct influence on the initiation and evolution of microstructural damage, which is also sensitive to the presence of imperfections, flaws or porosity.

The microstructure of polycrystalline materials, and its failure mechanisms, can be investigated using experimental [2] and computational [3] techniques. However, a truly three-dimensional (3D) experimental characterization still poses relevant challenges; on the other hand, the present-day availability of cheaper and more powerful computational resources and facilities, namely High Performance Computing (HPC), is favoring the advancement of *Computational Micromechanics* [4].

The explicit simulation of the material microstructure and its evolution finds a remarkable application in the *multiscale analysis of solids*, in which a considered component is analyzed simultaneously at the *component level*, for which the load history is defined, and at the *grain scale level*, which provides the constitutive material evolution. The term multiscale can assume a variety of meanings [5]: however, here we focus on simulations involving two spatial scales, the continuum level and the grain scale level. The objective of these studies is the analysis of both the behavior of the macro-component and the processes happening at the microscale during the loading history. The multiscale analysis becomes particularly useful when, during the loading history, the microstructure undergoes transformations or damage, so that a simple constitutive model assumed at the macro-level could not be used to simulate the behavior of the structure.

In this work a fully three-dimensional two-scale boundary element approach to degradation and failure in polycrystalline materials is proposed. At the macroscale, the damage-induced local softening is modelled employing a classical *initial stress approach*, while the microscopic degradation processes are explicitly modelled employing a cohesive-frictional three-dimensional grain-boundary formulation to simulate *intergranular* degradation and failure in the microstructural Voronoi-type morphology [2,6]. The strategies for coupling the two scales as well as avoiding pathological damage localization at the macroscale are briefly described. Some preliminary results are eventually discussed.

Two-scale formulation for polycrystalline degradation and failure

Macroscale model. The component level is described using a classical non-linear incremental 3D BEM formulation, where the presence of regions experiencing material softening, due to microstructural degradation, is taken into account introducing an *initial stress approach* [7,8]. The *total macro-stress* tensor components at a macroscopic material points are given by

$$\dot{\Sigma}_{ij} = \dot{\Sigma}_{ij}^{el} - \dot{\Sigma}_{ij}^{D} = C_{ijlk}\dot{\Gamma}_{ij} - \dot{\Sigma}_{ij}^{D} \tag{1}$$

where $\dot{\Sigma}_{ij}^{D}$ are the components of the *decremental macro-stress* tensor contributing to the *total macro-stress* components $\dot{\Sigma}_{ij}$ by reducing the value of the *elastic macro-stress* components $\dot{\Sigma}_{ij}^{el}$ that would correspond to the *local macro-strain* components $\dot{\Gamma}_{ij}$ in absence of damage. The boundary integral equation used to model the macro-scale is

$$c_{ij}(\mathbf{x})\dot{u}_j(\mathbf{x},\mathbf{y}) + \int_S T_{ij}(\mathbf{x},\mathbf{y})\cdot\dot{u}_j(\mathbf{y})\cdot dS = \int_S U_{ij}(\mathbf{x},\mathbf{y})\cdot\dot{t}_j(\mathbf{y})\cdot dS + \int_{V_D} \Psi_{ijk}(\mathbf{x},\mathbf{Y})\cdot\dot{\Sigma}_{jk}^{D}(\mathbf{Y})\cdot dV \tag{2}$$

where the last integral is performed over internal regions experiencing damage evolution. At a given macro-step, associated with a distribution of internal damage, Eq.(2) provides the values of boundary displacements and tractions that are subsequently used to compute the *macro-strain components* through the integral equation [7,8]

$$\dot{\Gamma}_{ij}(\mathbf{X}) + \int_S T_{ijk}^{\gamma}(\mathbf{X},\mathbf{y})\cdot\dot{u}_k(\mathbf{y})\cdot dS = \int_S U_{ijk}^{\gamma}(\mathbf{X},\mathbf{y})\cdot\dot{t}_k(\mathbf{y})\cdot dS + \int_{V_D} \Psi_{ijlk}^{\gamma}(\mathbf{X},\mathbf{Y})\cdot\dot{\Sigma}_{lk}^{D}(\mathbf{Y})\cdot dV + f_{ij}^{\gamma}\left[\dot{\Sigma}_{lk}^{D}(\mathbf{X})\right] \tag{3}$$

The macro-strain components at an internal macro-point **X** are subsequently used as boundary conditions for the corresponding associated micro-RVE. However, the direct use of the components $\dot{\Gamma}_{ij}$ provided by Eq.(3) may induce pathological localization of damage at the macro-scale. For this reason, a non-local integral counterpart of $\dot{\Gamma}_{ij}$, denoted here with $\hat{\dot{\Gamma}}_{ij}$, is used for providing the RVE boundary conditions, ensuring uniqueness and reproducibility of results. The terms $\dot{\Sigma}_{ij}^{D}$ in Eqs.(2-3) are provided by suitable homogenization performed over the micro-scale RVEs, as will be shown.

Microscale model. The micro-scale grain boundary formulation employed for following the micro-structural material degradation is described in detail in [2,6]. Here, it is briefly recalled for the sake of completeness. The microstructure morphology is generated using Voronoi tessellations. Each grain is modeled as a 3D linear elastic orthotropic domain with arbitrary spatial orientation, using the BEM for 3D anisotropic elasticity [9]. The polycrystalline aggregate is seen as a multi-region problem [2]. Given a volume bounded by an external surface and containing N_g grains, two kinds of grains can be distinguished: the *boundary grains*, intersecting the external boundary, and the *internal grains*, completely surrounded by other grains. Boundary conditions are prescribed on the surface of the boundary grains lying on the external boundary, while interface equations and equilibrium conditions are forced on interfaces between adjacent grains, to restore the integrity of the aggregate. The boundary integral equation for a generic grain $\mathcal{G}_k$ is written

$$\tilde{c}_{ij}^{k}(\boldsymbol{x})\tilde{u}_{j}^{k}(\boldsymbol{x})+\int_{B_C\cup B_{NC}}\tilde{T}_{ij}^{k}(\boldsymbol{x},\boldsymbol{y})\tilde{u}_{j}^{k}(\boldsymbol{y})dB^{k}(\boldsymbol{y})=\int_{B_C\cup B_{NC}}\tilde{U}_{ij}^{k}(\boldsymbol{x},\boldsymbol{y})\tilde{t}_{j}^{k}(\boldsymbol{y})dB^{k}(\boldsymbol{y}) \tag{4}$$

where $\tilde{u}_j^k$ and $\tilde{t}_j^k$ represent components of displacements and tractions of points belonging to the surface of the grain $\mathcal{G}_k$, the tilde refers to quantities expressed in a local reference system set on the grain surface, $\tilde{U}_{ij}^k$ and $\tilde{T}_{ij}^k$ are the 3D displacement and traction fundamental solutions for the anisotropic elastic problem.

The integrals in Eq.(4) are defined over the surface of the grain, that is generally given by the union of *contact* interfaces B_C and external *non-contact* surfaces B_{NC}. The model for the polycrystalline aggregate is obtained by discretizing Eq.(4) for each grain and complementing the system so obtained with a set of suitable *boundary* and *interface equations*. The interface between two grains can be either *pristine, damaged* or *failed*. When an interface is pristine continuity equations hold. Damage is introduced at the interface when the value of a suitable *effective traction* overcomes the *interface cohesive strength* $T_{\max}$ [6]. When such condition is fulfilled, the following traction-separation laws are introduced at the interface

$$\begin{bmatrix}\tilde{t}_1\\ \tilde{t}_2\\ \tilde{t}_3\end{bmatrix}=\frac{T_{\max}\left(1-d^*\right)}{d^*}\begin{bmatrix}\alpha/\delta u_t^c & 0 & 0\\ 0 & \alpha/\delta u_t^c & 0\\ 0 & 0 & 1/\delta u_n^c\end{bmatrix}\begin{bmatrix}\delta\tilde{u}_1\\ \delta\tilde{u}_2\\ \delta\tilde{u}_3\end{bmatrix};\qquad d^*=\max_{Load\ Hist}\left\{d=\left[\left\langle\frac{\delta u_n}{\delta u_n^c}\right\rangle^2+\beta^2\left(\frac{\delta u_t}{\delta u_t^c}\right)^2\right]^{\frac{1}{2}}\right\} \tag{5}$$

where $d^*\in[0,1]$ is an *interface damage parameter*, δu_n and δu_t are the normal and tangential interface opening displacements and δu_n^c and δu_t^c represent their critical values in pure mode I and II respectively and *d* is the *effective opening displacement*. Upon interface failure, the traction-separation laws are replaced by the laws of the *frictional contact mechanics*. After discretization and classical BEM implementation of Eqs.(4) and the associated boundary and *evolving* interface conditions a sparse system is obtained and an *incremental/iterative algorithm* is employed to track the microstructural evolution. A load increment is applied and the system solution is iterated until no violation of the interface equations is detected and convergence is then reached. The interested reader is referred to [6] for further details about the micro-structural model.

Scales coupling: down-scaling and up-scaling. The macro- and micro-scale models must be suitably coupled to capture the damage evolution. The macro-scale may be representative of an engineering component or coupon, which is progressively loaded by external loads. Boundary conditions are defined at this level as a problem input in terms of a macro load factor Λ. The macro-component is assumed initially pristine and no macro-damage is present. When the initial elastic problem is solved, the internal points experience a macroscopic strain field $\dot{\Gamma}_{ij}$ that can be computed through Eq.(3). Such strain field provides the boundary conditions for the micro-RVEs associated with the relevant internal points. Different kind of boundary conditions can be applied to the RVEs: in this work the macro-strains are used to provide *periodic micro boundary conditions* expressed by

$$\dot{u}_i^S=\dot{u}_i^M+\dot{\hat{\Gamma}}_{ij}\cdot\left(x_j^S-x_j^M\right);\qquad \dot{t}_i^S=-\dot{t}_i^M \tag{6}$$

where the hat expresses non-local counterparts of the local macro-strains. Eqs.(6) express the *downscaling* of the macro-strains. Once periodic BCs coming from the macro-scale simulation are available to the micro-RVEs, the micro-scale simulations can start. From a threshold value of the macro load factor on, some RVEs start experiencing microstructural damage. The micro-structural damage is reflected at the macro-scale by some *local softening*. To define the macro-damage, i.e. *to up-scale damage*, the following technique is employed. Given a generic RVE subjected to some macro-strain periodic BCs $\dot{\hat{\Gamma}}_{ij}$, it is possible to associate a macro-stress measure to $\dot{\hat{\Gamma}}_{ij}$ through computational homogenization:

$$\dot{\Sigma}_{ij}=\left\langle\dot{\sigma}_{ij}^{\mu}\right\rangle=\frac{1}{V^{\mu}}\int_{V^{\mu}}\dot{\sigma}_{ij}^{\mu}dV^{\mu}=\frac{1}{S^{\mu}}\int_{V^{\mu}}x_i\cdot t_j^{\mu}dV^{\mu} \tag{7}$$

where the integrals are defined over the RVE volume. If the RVE is pristine, the value of macro-stress should coincide with that obtained by the elastic material effective properties (overall properties), i.e. $\dot{\Sigma}_{ij}^{el}$. On the other hand, if micro-damage is present, the macro-stress will be degraded. The degradation is expressed, in the present model, through the decremental component of stress

$$\dot{\Sigma}_{ij}^{D} = \dot{\Sigma}_{ij}^{el} - \dot{\Sigma}_{ij} = \left(1 - \frac{\dot{\Sigma}_{ij}}{\dot{\Sigma}_{ij}^{el}}\right)\dot{\Sigma}_{ij}^{el} = D_{ij} \cdot \dot{\Sigma}_{ij}^{el} \tag{8}$$

where $0 \le D_{ij} \le 1$ is a macroscopic damage coefficient expressing the degradation of the material at the macro-point associated with the considered RVE. To determine the damage coefficient then the following practical stress are followed: *a*) a suitable measure of macro-strain is down-scaled; *b*) the micro-RVEs are simulated; *c*) the macro-stress components $\dot{\Sigma}_{ij}$ are computed and compared with $\dot{\Sigma}_{ij}^{el}$ to estimate macro-damage D_{ij}; *d*) the macro-damage is used to define the decremental components of macro-stress.

Macro-micro algorithm. The solution of the two-scale problem involves an incremental-interative macro-micro iterative solution strategy, which is briefly discussed here. The analysis starts with the determination of the macro load factor that initiates micro-structural damage. From then on, the analysis is fully non linear. The macro-strain field is downscaled and provides periodic BCs for the micro-RVEs. The microstructural RVEs are simulated and a macro-damage measure is defined for each active RVE though homogenization. The macro-damage is then used to compute the components of the decremental stress used in Eqs.(2-3). Convergence is checked by assessing the convergence of macro internal energy for each relevant macro-cell experiencing damage. When a micro-RVE is too damaged, the corresponding macro-cell is removed and a macro-crack is initiated. The two-scale analysis strategy is illustrated in Fig.(1).

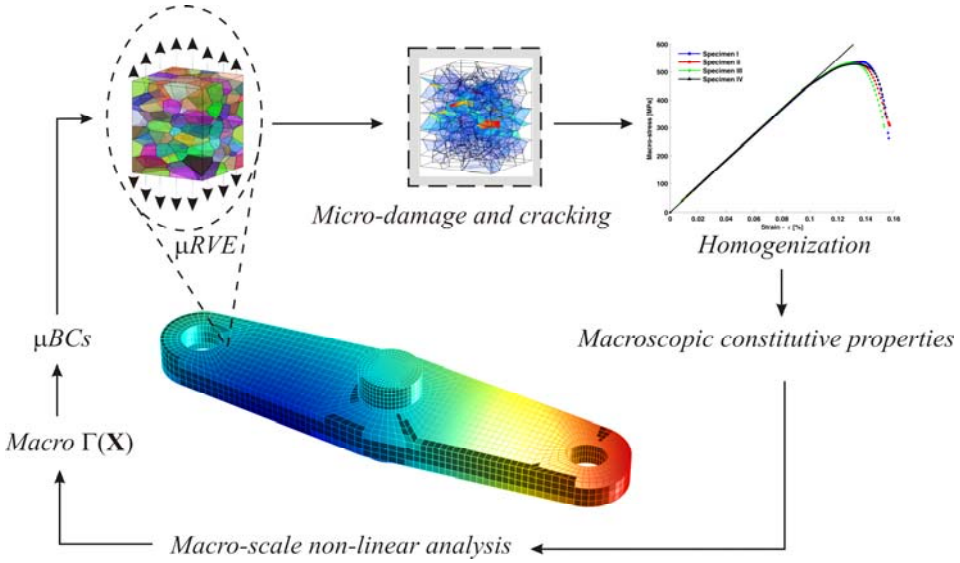

Fig. 1: Multiscale analysis scheme: the macro-scale analysis provides the boundary conditions for the micro-RVEs, whose evolution provides the constitutive behaviour for the macro-scale.

Some preliminary numerical results

Some qualitative preliminary results are reported here. One of the main challenges, when dealing with fully 3D multiscale simulations, is the computational burden of the analysis. Several simulations are currently being carried out to test the capability of the formulation and complete results will be reported soon. However, some partial results are shown here, mainly to illustrate the aim of the method.
The analyzed structural macro-scale component is depicted in Fig.(2), where also the specimen size, mesh features and macro-scale boundary conditions are given. The specimen is loaded in displacement control.

Micro-scale data. The considered material is polycrystalline alumina. In Voigt notation, for the alumina single crystals, the elatsic constant (to be used in the micro-model, are: $C_{11} = 496.8$ GPa, $C_{12} = 163.6$ GPa, $C_{13} = 110.9$ GPa, $C_{14} = -23.5$ GPa, $C_{33} = 498.1$ GPa, $C_{44} = 147.4$ GPa. The grain size is ASTM $G = 10$. The cohesive-frictional inter-granular properties [6] are: $K_{IC} = 4$ MPa$\cdot$m$^{1/2}$, $T_{\max} = 500$ MPa, $\alpha = \beta = 1$, $\mu = 0.2$. Micro-RVEs with 20 grains are considered.

Macro-scale data. The considered macro-mesh has $15 \times 8 \times 4$ volume macro-cells, with the corresponding associated micro-RVEs. The macro-scale material properties are $E = 407$ GPa and $\nu = 0.24$.

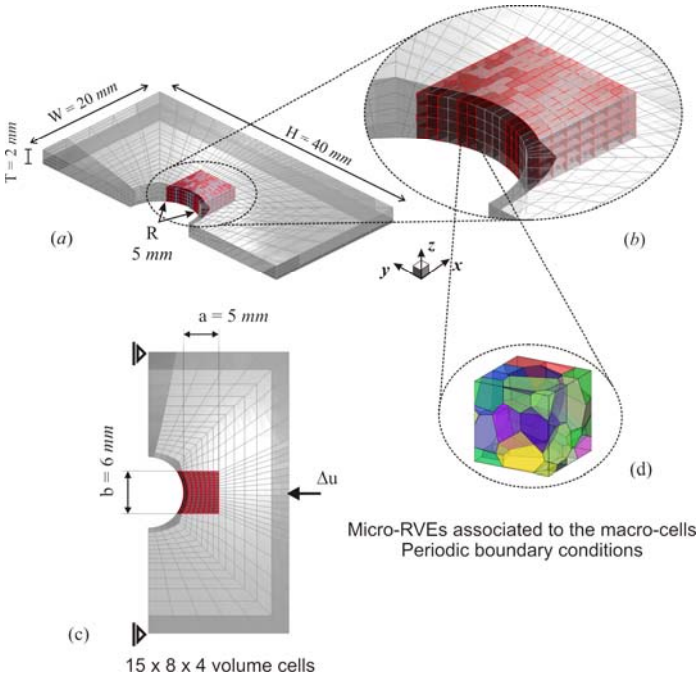

Fig. 2: Scheme of the performed numerical test.

Fig.(3) reports the distribution of macro-damage after 80 complete load increments, completed after approximately five days on 12 core machines. The relative magnitude of damage is shown. Few observation are worth. The color intensity is proportional to $\max_{i,j}\left(D_{ij}\right)$ in Eq.(8) for the macro-points associated with the micro-RVEs. The absolute damage values are very low and associated mainly with shear loads acting on the micro-RVE. The different behavior of the RVEs to shear acting in opposite directions explains also the apparent lack of symmetry in damage distribution. It is expected that the lack of symmetry will be overcome at higher values of damage. Moreover, no removal of macro-cells occurs within the simulated range, as the damage has not reached critical values in any internal point.

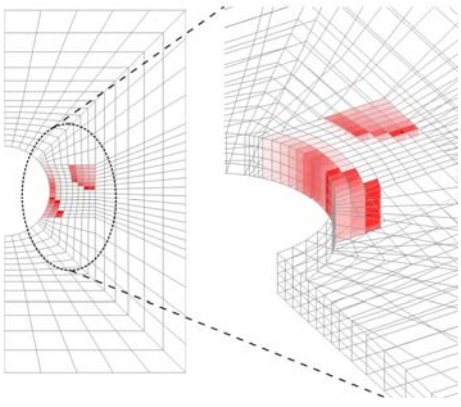

Fig. 3: Damage activation after 80 macro-micro increments.

An important parameter in the simulations is the number of grains used in the RVEs: the lower limit is imposed by considerations of material representativity of the microstructure; the upper limit, at least in the present framework, is imposed by the need of maintaining acceptable computational requirements. The effect of this and other parameters is being currently investigated in on-going multiscale simulations.

Summary

A two-scale three-dimensional framework for degradation and failure of polycrystalline material engineering components has been presented. The formulation is quasi-static and fully three-dimensional. The macroscale accounts for the presence of material damage by using a classical boundary element incremental initial stress approach, analogous to the method used in elasto-plastic analyses. The three-dimensional micro-RVEs are analyzed employing a three-dimensional grain-boundary cohesive-frictional approach. The coupling between the two scales is achieved downscaling macro-strains as periodic RVE boundary conditions and up-scaling damage through volume stress averages. Some preliminary results are shown to illustrate the aim of the technique. Intensive simulations on several aspects and challenging issues are currently being carried out, to highlight the capability of the technique.

Acknowledgements

This research was partially supported by a Marie Curie Intra-European Fellowship within the 7th European Community Framework Programme (Project No 274161).

References

[1] S. Nemat-Nasser, M. Hori, *Micromechanics: overall properties of heterogeneous materials*, North-Holland, Elsevier, The Netherlands, second revised edition edition, (1999).

[2] I. Benedetti, M. H. Aliabadi, A three-dimensional grain boundary formulation for microstructural modelling of polycrystalline materials, *Computational Materials Science*, **67**, 249–260, (2013).

[3] T. I. Zohdi, P. Wriggers, *An introduction to computational micromechanics*, Lecture Notes in Applied and Computational Mechanics, vol. 20, Springer, Berlin, (2005).

[4] I. Simonovski, L. Cizelj, Computational multiscale modeling of intergranular cracking, *Journal of Nuclear Materials*, **414**, 243 – 250, (2011).

[5] Ghoniem, N. M., Busso, E. P., Kioussis, N., Huang, H., Multiscale modelling of nanomechanics and micromechanics: an overview, *Philosophical magazine*, **83**(31-34), 3475-3528, (2003).

[6] Benedetti, I., Aliabadi, M.H., A three-dimensional cohesive-frictional grain-boundary micromechanical model for intergranular degradation and failure in polycrystalline materials. Computer Methods in Applied Mechanics and Engineering, **265**, 36-62, (2013).

[7] P.K. Banerjee, *The boundary element methods in engineering*, McGraw-Hill, 1994.

[8] M.H. Aliabadi, The boundary element method: applications in solids and structures., Vol. 2, John Wiley & Sons Ltd, England, (2002).

[9] R.B. Wilson, T.A. Cruse, Efficient implementation of anisotropic three-dimensional boundary-integral equation stress analysis, *International Journal for Numerical Methods in Engineering*, **12**, 1383–1397, (1978).