Author's checklist

- ☐ I followed TTP's author-instructions/sample-article.
- ☐ I set the page settings of my word processor to the A4 format; with the margins: bottom 1.5 cm and top 2.5 cm or bottom 0.6 in and top 1 in. (**We shall be able to produce a pdf file from your paper only if the paper format and the margins are correct.)**
- ☐ I used good-quality white paper of approximately 21 x 29.7 cm or 8.2 x 11.6 in to print my paper *(please do not change the document setting from A4 to any other format as the article will print satisfactorily onto either of the above-mentioned paper sizes).*
- ☐ I sent an identical electronic file (RTF, MS Word, LaTex) together with the hardcopy. (If the paper size and page set-up are not as described above, we shall be unable to publish your paper in electronic form on our web page: http://www.scientific.net. We shall then have to scan it which, when compared with an electronic version, results in very poor quality.)
- ☐ I have always used the same version of the name(s) (i.e. either F.A. Miller or Fred A. Miller or Fred Miller but not various versions alternately), as only the exact agreement of email and name will allow me to access my paper on the web.
- ☐ I included my email address and email addresses of co-authors in the paper.
- ☐ I filled out and signed the proper copyright transfer agreement *(mandatory).*
- ☐ **I sent all of the above-mentioned documents to the corresponding editor**

- ☐ I filled out an offprint order form.
- ☐ I included color pictures and wish to have these printed in full color. Please bill me the additional charge of Euro 980.00 per *page (must be prepaid).*
    - ☐ I would like to also order _____ offprints *(these must be ordered before printing we will send you an invoice, post-printing orders will be reproduced in black and white only)*

    Name/signature_____

    Date _____

Please transmit color page charges to

Credit Suisse, Branch Meilen, 8706 Meilen, Switzerland, Clearing No. 4823: Account No. 339209-92-1, SWIFT Code: CRESCHZZ63A, IBAN CH60 0482 3033 9209 9200 1
Or: Postal Checking Account: No. 45-982.1, Solothurn, Switzerland
Our VAT No.: MWST 265 430

A multiscale approach to polycrystalline materials damage and failure

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 damage modelling; Micromechanics; Boundary element method.

Abstract. A two-scale three-dimensional approach for degradation and failure in polycrystalline materials is presented. The method involves the component level and the grain scale. The damage-induced softening at the macroscale is modelled employing an *initial stress boundary element approach*. The microscopic degradation is explicitly modelled associating Representative Volume Elements (RVEs) to relevant points of the macro continuum and employing a cohesive-frictional 3D grain-boundary formulation to simulate *intergranular* degradation and failure in the Voronoi morphology. Macro-strains are *downscaled* as RVEs' periodic boundary conditions, while overall macro-stresses are obtained *upscaling* the micro-stress field via volume averages. The comparison between effective macro-stresses for the damaged and undamaged RVEs allows to define a macroscopic measure of local 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

The prediction of materials degradation and failure is relevant for several structural applications and it is recognized that the macroscopic material properties depend on the material microstructure[1].

Polycrystalline materials, either metals, alloys or ceramics, are commonly employed in engineering and their degradation is influenced, at the microscopic level, by grains morphology, size distribution, anisotropy and crystallographic orientation, stiffness and toughness mismatch and by physical and chemical properties of the intergranular interfaces. These features, and their effect on the macro-properties, can be investigated using experimental [2] and computational [3] techniques. The present-day availability of more powerful computational resources and facilities, namely High Performance Computing, is promoting the advancement of *Computational Micromechanics* [4].

The explicit simulation of the micro-structure has remarkable application in the *multiscale analysis of solids*. The term multiscale may assume a variety of meanings: however, here we focus on simulations involving two spatial scales, the *component level* and the *grain level*. The objective of these studies is modelling the constitutive behavior without explicit assumptions at the macro-scale: the constitutive behavior emerges from simulations at a scale below the considered one, where fewer approximations may be introduced. The approach is particularly useful when a simple macro-constitutive model cannot be assumed, e.g. when transformations or damage are present.

In this work, a two-scale fully 3D boundary element approach to polycrystalline degradation 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 [2,5]. The strategies for coupling the two scales and avoiding pathological damage localization at the macroscale are briefly described. Some preliminary results are eventually discussed.

Multiscale formulation

Macroscale model. The macro-level is modelled through a non-linear incremental 3D boundary element formulation, where material softening, due to microstructural degradation, is taken into account introducing an *initial stress approach* [6,7]. The *total macro-stresses* at a macro-point are defined by

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

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

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

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 [6,7]

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

The macro-strains at an internal macro-point **X** are subsequently downscaled 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 $\dot{\Sigma}^{D}_{ij}$ in Eqs.(2-3) are provided by suitable homogenization performed over the micro-scale RVEs, as it will be shown.

Microscale model. The micro-scale grain-boundary formulation is described in detail in [2,5]. Here, it is briefly recalled for the sake of completeness. The microstructure morphology is a Voronoi tessellation. Each grain is a 3D linear elastic anisotropic domain with arbitrary spatial orientation, and it is modelled through BEM for 3D anisotropic elasticity [8]. The aggregate is seen as a multi-region problem [2]. The boundary integral equation for a generic grain $\mathcal{G}_k$ is written

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

where $\tilde{u}^{k}_{j}$ and $\tilde{t}^{k}_{j}$ 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, $\tilde{U}^{k}_{ij}$ and $\tilde{T}^{k}_{ij}$ are the 3D displacement and traction fundamental solutions for the anisotropic elastic problem.

Eq.(4) is defined over the surface of the grain, generally given by the union of *contact* interfaces B_C and external *non-contact* surfaces B_{NC}. The model for the aggregate is obtained by discretizing Eq.(4) for each grain and complementing the system with a set of *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* $T_{\max}$ [5]. When such condition is fulfilled, the following traction-separation laws are introduced at the interface

$$\tilde{\mathbf{t}} = \mathbf{K}\left(T_{\max}, d^*, \delta u_t^c, \delta u_n^c\right) \cdot \delta\tilde{\mathbf{u}}; \qquad d^* = \max_{Load\ Hist}\left\{ d = \sqrt{\left\langle \delta u_n / \delta u_n^c \right\rangle^2 + \beta^2 \left(\delta u_t / \delta u_t^c \right)^2} \right\} \tag{5}$$

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. Details in [5].

Scales coupling. The macro- and micro- scales must be suitably coupled. The macro-component is initially pristine and no damage is present. Under external loads, the internal points experience macroscopic strains $\dot{\Gamma}_{ij}$, which can be computed through Eq.(3) and provide the boundary conditions for the micro-RVEs. In this work *periodic boundary conditions* are implemented for the RVEs. Once the RVEs' BCs coming from the macro-scale simulatiosn are available, the micro-scale can be simulated. Starting from a threshold value, damage initiates in some RVEs. The micro-damage is reflected at the macro-scale by *local softening*. To define the macro-damage, i.e. *to up-scale damage*, volume stress averages for the damaged RVEs are computed and used to compute the components of decremental stess $\dot{\Sigma}_{ij}^D$ for the macro-point associated with the RVE.

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 that moment on, the analysis is fully non linear. The macro-strains provide periodic BCs for the micro-RVEs. The micro-RVEs are simulated and macro-damage is defined for each active RVE through homogenization. The macro-damage is then used to compute the decremental stresses used in Eqs.(2-3). Convergence is checked by assessing the convergence of internal energy at the macro-level. 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).

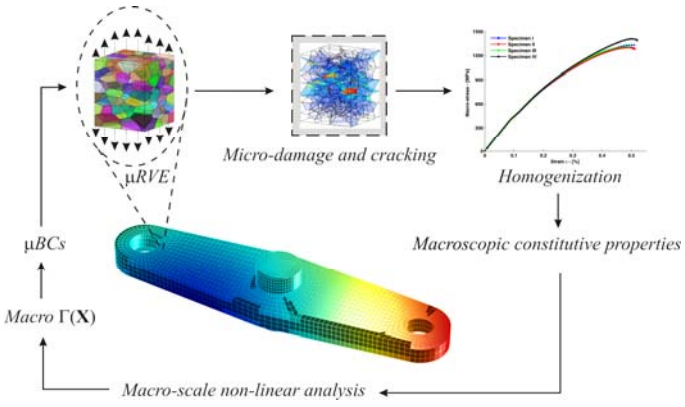

Fig. 1: Multiscale analysis scheme: the macro- analysis provides the boundary conditions for the micro-RVEs, whose simulation provides the constitutive behaviour for the macro-scale.

Some preliminary numerical results

Some preliminary results are reported. A relevant challenge of the fully 3D multiscale method is the computational burden. Several simulations are currently being carried out to test its capability However, some preliminary results are shown to illustrate the method’s aim.

The analyzed macro-scale component is shown in Fig.(2), where also the specimen size, loading 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 elastic constants 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 [5] are: $K_{IC} = 4$ MPa$\cdot$m$^{1/2}$, $T_{\max} = 500$ MPa, $\alpha = \beta = 1$, $\mu = 0.2$. Micro-RVEs with 20 and 40 grains are considered.

Macro-scale data. The considered macro-meshes have $15 \times 8 \times 4$ (mesh A) and $17 \times 10 \times 4$ (mesh B) volume macro-cells, with the corresponding associated micro-RVEs. The macro-scale material properties are $E = 407$ GPa and $\nu = 0.24$.

Fig.(2) shows the macro-damage distribution for four different tests. Tests A and B involve the smaller and larger macro-meshes, respectively, with 20 grains per RVE. Tests C and D involve the smaller and larger macro-meshes, respectively, but with 40 grains per RVE. For all tests, 240 hours elapsed time has been set, so that simulations with smaller RVEs have attained larger macro-load factors. The four macro-damage snapshots correspond to the macro load factors: $\Lambda_A = 0.817994\text{E-}01$; $\Lambda_B = 0.799908\text{E-}01$; $\Lambda_C = 0.651501\text{E-}01$; $\Lambda_D = 0.635259\text{E-}01$. Preliminary results appear consistent.

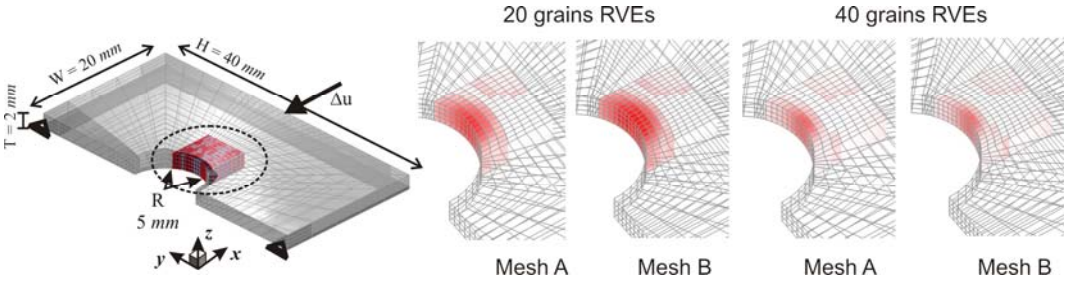

Fig. 2: Macro-damage patterns for the performed tests.

Summary

A two-scale framework for degradation in polycrystalline materials is presented. The formulation is quasi-static and fully three-dimensional. The macroscale accounts for the presence of damage through a boundary element incremental initial stress approach. The micro-RVEs are analyzed using a grain-boundary cohesive-frictional approach. The macro-strains provide periodic boundary conditions for the micro-RVEs and micro-damage is up-scaled through volume stress averages. Some preliminary tests are shown to illustrate the aim of the technique. Several aspects and challenges of the method are currently under investigation.

References

[1] S. Nemat-Nasser, M. Hori, *Micromechanics: overall properties of heterogeneous materials*, (North-Holland, Elsevier, The Netherlands, 1999).
[2] I. Benedetti, M.H. Aliabadi: Comput Mater Sci, Vol. 67, (2013), p. 249.
[3] T.I. Zohdi and P. Wriggers: *An introduction to computational micromechanics*, (Springer, Berlin, 2005).
[4] I. Benedetti & F. Barbe, *Modelling Polycrystalline Materials: An Overview of Three-Dimensional Grain-Scale Mechanical Models*. Journal of Multiscale Modelling, (2014).
[5] I. Benedetti, M.H. Aliabadi: Comput Meth Appl Mech Eng, Vol. 265, (2013), p. 36.
[6] P.K. Banerjee: *The boundary element methods in engineering*, (McGraw-Hill, 1994).
[7] M.H. Aliabadi, *The boundary element method: applications in solids and structures*, (John Wiley & Sons Ltd, England, 2002).
[8] R.B. Wilson, T.A. Cruse, *Int J Numer Meth Eng*, Vol. 12, (1978), p. 1383.