A MULTI-SCALE "MORPHOLOGICAL APPROACH" FOR MODELING THE NON LINEAR BEHAVIOR OF PROPELLANT-LIKE MATERIALS

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Abstract

This paper deals with a non-classical scale transition, called "morphological approach" (MA), for modeling the non linear behavior of highly-filled particulate composites. In particular, it focuses on damage by grain/matrix debonding. The modeling proposed by Nadot et al [1], by extension in the presence of damage (fixed state) of the approach initially proposed by Christoffersen [2], is here completed with ingredients allowing to describe damage evolution. A defect nucleation criterion and a closure criterion are formulated at the local scale. The formulation takes advantage of the morphological insight of the MA and of the direct accessibility to an estimate of the local displacement. The modeling thus enhanced allows to follow damage evolution as a discrete sequence of interfacial debonding including also eventual closure of defects. A numerical illustration shows the ability of the MA to describe damage characteristics (chronology of events, position and morphology of microdefects) as well as its macroscopic consequence (induced anisotropy and unilateral effects).

1 Introduction and scope

This study is part of a long-time research program aiming at predicting the vulnerability of energetic composites, such as propellant-like materials. These materials are constituted of a high proportion (> 60% in volume) of irregular energetic crystal grains randomly distributed in a rubber-like matrix. It is well known that microscopic damage occurring during a first loading path may increase drastically the sensitivity of such materials. They may become dangerous when submitted to a second loading even for moderate strain rates. Indeed interfacial defects (pores) or intergranular microcracks may be the location of local chemical reactions leading to the initiation and propagation of combustion within the material. These reactions are moreover influenced by local heat due to mechanical dissipation inherent to damage micromechanisms. Nowadays, reactive models exist in order to predict such events and more generally unexpected non nominal behaviors (*e.g.* deflagration, detonation). Nevertheless, they require the knowledge of essential data that have to be provided by efficient micromechanical models. These data concern the damage configuration in the material (position and morphology of microdefects) and also the estimate of local strain and stress fields. To this end a specific multi-scale modeling is here proposed.

Considering the complex mechanical behavior of propellant-like materials involving strong coupling between several non linear mechanisms (finite strain viscoelasticity, damage by grain matrix/debonding for quasi-static loading paths, microcracking of grains for dynamic loadings…), the advanced multi-scale modeling has been developed using a progressive, step-by-step, approach of difficulties. The latter is based on a methodology initially proposed by Christoffersen [2] for linear elastic highly-filled particulate composites which has been first extended to account for the small strain viscoelasticity of the matrix [3]. More recently, it has been also extended in finite strain hyperelaticity [4] and viscohyperelasticity [5], [6]. Actually, damage by grain matrix/debonding for quasi-static loading paths is introduced into the multi-scale framework [1]. The specificity of the MA lies notably in a *direct* and explicit geometrical schematization of the real random microstructure adapted to the high volume fraction of particles. The coupling between this morphological insight and a local kinematics postulated (assumptions regarding notably matrix related displacement field) makes the MA able to provide a direct accessibility to an estimate of local fields, as required by the application, in addition to that of the homogenized response. This feature remains valid whatever are the constituents' behaviors. Moreover, some rich and relevant information concerning morphology and internal arrangement of the constituents is taken into account explicitly in the local and global estimates, via the geometrical parameters defined during the first schematizing step. In particular, the estimated strain field in the matrix, softer than the grains, is strongly influenced by global, but also, by local morphology (that of the neighborhood of the considered point) and eventually by local damage events. Such a local heterogeneity is taken into account in the homogenized behavior estimate. This is essential considering the important effect of local heterogeneity on the non linear macroscopic behavior as shown for example by [7], [8]. Thus, the double schematization proper to MA allows a *direct* approach of field fluctuations in the matrix via the morphological parameters. From a general viewpoint, it is to be noted that a fair description of a representative volume element (R.V.E.) has always been a key issue in the context of "averaging methods" [9]. For the application at stake, taking into account local morphology in the matrix strain field estimate is an essential advantage considering the strong influence of local morphology on damage micromechanisms. The present paper focuses on the presentation of the MA in its version including damage by grain/matrix debonding. For applications of the MA to sound viscohyperelastic composites, the interested reader may refer to the works [5], [6] and [10]. The quality of local and global estimates is evidenced through comparisons with results obtained by full-field simulations. This is done for a specific periodic microstructure (see [6]) and for a real random propellant-like material (see [10]). The MA is shown to provide good results for a CPU time much lower than the one required by finite element calculations. In [10], the MA homogenized response for a hydrostatic loading path is also confronted to experience.

In Section 2, the principal ingredients of the MA (*direct* schematization of the microstructure, different stages of the solving procedure for a fixed number of open and closed defects) are first presented following [1]. Then, analytical results obtained at both scales for elastic linear constituents (grains and matrix) are described as an illustration of the effects captured by the MA. Section 3 deals with the description of damage evolution by the formulation of two local criteria (nucleation and closure of defects) exploiting the direct characterization of the interfaces and the knowledge of the local displacement field as a function of the morphology around the interfaces. Finally, Section 4 gives a numerical illustration of the ability of the MA to deal with damage evolution in a random three-dimensional composite containing 400 grains submitted to a complex loading path. The homogenized response is discussed with special attention paid on the evolution of the damage induced anisotropy as a function of the chronology of local damage events (discrete sequence of nucleations and closures). The ability of the MA to give access to the position and morphology of microdefects, according to the requirements of the application context, is illustrated through 3D representations of the damaged microstructure.

2 Morphological approach in presence of damage (fixed state)

2.1 Direct geometrical schematization

The initial random microstructure of a highly filled composite is represented by an aggregate of polyhedral grains interconnected by thin matrix layers with constant thicknesses. This schematization is illustrated in figure 1. For each layer α, a set of four "morphological parameters" is identified in the non-deformed configuration:

- h^α, the constant thickness of layer α
- A^α, the projected area of layer α; the associated volume is then $A^\alpha h^\alpha$
- $\boldsymbol{d}^\alpha$, the vector linking the centroids of the polyhedra separated by layer α
- $\boldsymbol{n}^\alpha$, the unit vector normal to the plane interface grain/layer α.

Once the grains are replaced by polyhedra (satisfying the condition of parallelism between the interfaces of opposite grains), the parameters $\boldsymbol{d}^\alpha$, $\boldsymbol{n}^\alpha$ and h^α are readily determined. The projected area A^α –leading to the definition of the matrix zone between two neighboring grains called "layer α"– is identified as follows. Starting from the centroids of the two grains, the two opposite interfaces are projected on the middle plane of the intergranular zone. Then, an average projection is defined and chosen as the area A^α. In this way, layer α (associated volume $A^\alpha h^\alpha$) does not correspond exactly to the matrix zone strictly confined between the two opposite interfaces. It can be larger as illustrated in Fig. 1c (2D representation). From a practical point of view, the challenge is to optimize the correspondence of the "true" microstructure with the schematized one in order to confer a fair relevance on the morphological parameters. X-ray tomography together with available tools of morphological analysis of 3D images may be used to this aim (see [10]). One may emphasize the direct character of such a schematization since each grain and each matrix intergranular zone are represented. The latter differs notably from e.g. the Eshelby-based self-consistent-like estimates. At last, one may note that the orientations of future interfacial defects are already predefined.

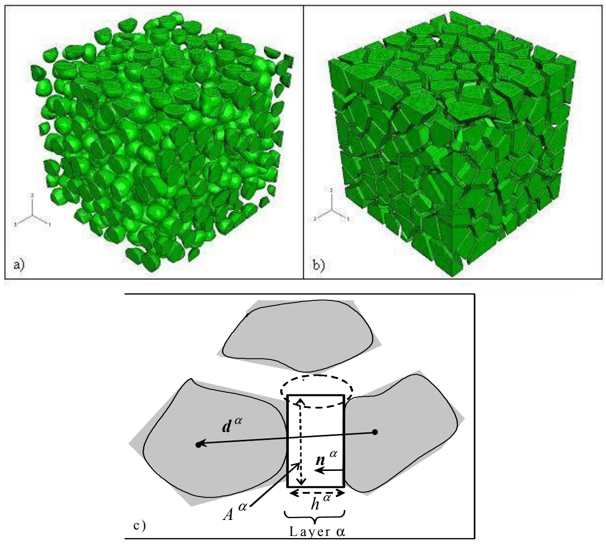


Fig. 1. Illustration of the geometrical schematization: a) real microstructure (X-ray tomography), b) schematized microstructure, c) morphological parameters for a layer α, [2].

2.2 Localization-homogenization problem: principal tools and stages

The second starting point of the MA consists in simplifying kinematical assumptions regarding the local displacement field in the schematized volume. They are recalled below. The grain centroids are displaced so as to conform to a global, homogeneous displacement gradient $\boldsymbol{F}$ (data for the local problem). The grains themselves are supposed homogeneously deformed and the corresponding displacement gradient $\boldsymbol{f}^0$ assumed to be common to all grains of the schematized volume. Each interconnecting layer is subjected to a homogeneous deformation, proper to the layer α under consideration and noted $\boldsymbol{f}^\alpha$. Local disturbances at grain edges and corners (see circled zone in Fig. 1c) are neglected on the basis of thinness of the layers. The interfacial defects and relative displacement jumps are incorporated in a compatible way with this kinematical description. In addition to imply the displacement jump linearity (affine defects, if any), the foregoing kinematical assumptions, and more precisely the second one regarding $\boldsymbol{f}^0$ as common to all grains, impose only two possible configurations for a layer α: either no decohesion, or simultaneous decohesion of its both interfaces. In order to make acceptable this

double decohesion (if any), a supplementary constraint to the geometrical schematization is added: any two opposite interfaces must have similar geometrical properties (shape and area). Furthermore and considering the parallelism of opposite interfaces in course of deformation, it is reasonable to consider that the mean displacement discontinuity vectors across the interfaces of a debonded layer α are opposite.
By taking into account conditions of displacement jump (with affine form for the jumps $b_i^\alpha = f_{ij}^{\alpha D} y_j$), the displacement gradient $\boldsymbol{f}^\alpha$ for a debonded layer α (*i.e.* with defects at its interfaces), is given by $(1)_1$. For a layer α whose both interfaces are cohesive $\boldsymbol{f}^\alpha$ is obtained by using the continuity of displacements on the grain/layer interfaces (see $(1)_2$):

$$f_{ij}^\alpha = f_{ij}^0 + \left(F_{ik} - f_{ik}^0\right) d_k^\alpha \; n_j^\alpha / h^\alpha + f_{ij}^{\alpha D} \quad (1)$$

$$f_{ij}^\alpha = f_{ij}^0 + \left(F_{ik} - f_{ik}^0\right) d_k^\alpha \; n_j^\alpha / h^\alpha$$

for layer α with no defect

The supplementary term $\boldsymbol{f}^{\alpha D}$ in $(1)_1$ represents the specific contribution of two interfacial defects located at the interfaces of the debonded layer α considered. The MA morphology and kinematic framework in the presence of damage allows to take into account some strain heterogeneity in the matrix phase governed by both local morphology and local damage events (see the dependence of $\boldsymbol{f}^\alpha$ on the morphological parameters proper to the layer α under consideration and on $\boldsymbol{f}^{\alpha D}$ for debonded layers). The compatibility between local motion defined above and the global one characterized by the given displacement gradient $\boldsymbol{F}$ (i.e. $\boldsymbol{F} = \langle \boldsymbol{f} \rangle_V$ + contribution of defects) is ensured through a geometrical condition to be satisfied by the morphological parameters of the schematized material, see [1] for detailed form and interpretation.
For a given number of open and/or closed defects, the unknown of the local problem $\boldsymbol{f}^0$ is deduced from the use of the generalized Hill lemma, by employing the local constitutive laws for the grains and the matrix and using the hypothesis of no sliding, *i.e.* infinite friction coefficient presumed on closed defect lips (see Section 3 in [1] for details). Finally, the knowledge of $\boldsymbol{f}^0$ allows the backwards calculation of the composite response at both scales: $\boldsymbol{f}^\alpha$ for any layer α by using (1), local stresses by the local constitutive laws and finally the homogenized stress tensor by volume averaging of the local one. The foregoing solving procedure remains valid whatever are the constituents' constitutive laws. It is analytical in the small strain framework. At this stage, it is nevertheless partial. Indeed, since nothing has been assumed regarding the detailed expression of the displacement jump in function of macroscopic displacement gradient $\boldsymbol{F}$ (except its linearity with respect to local spatial coordinate due to the kinematical description), local fields and homogenized stress will be expressed in function of the set $\{\boldsymbol{f}^{\alpha D}\}$. This offers an advantage to identify in an explicit way the contributions of defects in the expressions as illustrated by equation (4) in the next section. Evidently, a complementary stage, depending on the local behavior of constituents, is required to explicit some of the damage-induced quantities. In subsection 2.3, one analyses the results obtained for isotropic linear-elastic constituents (grains and matrix), framework in which a complementary localization-homogenization approach has been already proposed to the foregoing aim.
At last, one may note the direct character of the solving procedure that does not require any prior linearization of local non linear constitutive laws contrarily to more classical schemes referring to the notion of equivalent linear composite, see e.g. [11] for a review of existing linearization procedures.

2.3 Results in elasticity and complementary localization-homogenization approach

In the case of isotropic linear-elastic constituents (grains and matrix), the analytical expression of the local strain field and of the homogenized Cauchy stress tensor, resulting from the first stage of the scale transition according to the methodology summarized at the end of subsection 2.2, depend on the following quantities in addition to the elastic moduli of constituents:

$$\text{Global strain } \boldsymbol{E}=Sym.\ \boldsymbol{F} \qquad (2)$$

$$\left\{\boldsymbol{\varepsilon}^{\beta D};\ \beta\in L^{open}\right\},\quad \left\{\boldsymbol{\varepsilon}^{fD};\ f\in L^{closed}\right\}$$

$$\overline{T}_{ijkl}=\frac{1}{V}\sum_{\alpha} d_i^{\alpha}\ n_j^{\alpha}\ d_k^{\alpha}\ n_l^{\alpha}\ A^{\alpha}/h^{\alpha} \qquad (3)$$

$$D_{ij}=\frac{1}{V}\sum_{\beta\in L^{open}} d_i^{\beta} n_j^{\beta} A^{\beta}$$

$$\overline{D}_{ijkl}=\frac{1}{V}\sum_{\beta\in L^{open}} d_i^{\beta} n_j^{\beta} d_k^{\beta} n_l^{\beta} A^{\beta}/h^{\beta}$$

The strain of any layer α is also function of its morphological parameters according to (1). In the above equations, superscript α refers to any layer (debonded or not). L^{open}, respectively L^{closed}, represents the set of layers with open, respectively closed, defects at their interfaces. In accordance with $(1)_1$, the strain $\boldsymbol{\varepsilon}^{\beta D}=Sym.\ \boldsymbol{f}^{\beta D}$, respectively $\boldsymbol{\varepsilon}^{fD}=Sym.\ \boldsymbol{f}^{fD}$, represents for a layer $\beta\in L^{open}$, respectively $f\in L^{closed}$, the contribution to its 'total' strain of open, respectively closed, defects at its own interfaces. Moreover, the estimates account for initial morphology and internal organization of grains inside the volume through the presence of the fourth-order structural tensor $\overline{\boldsymbol{T}}$ given by $(3)_1$. The reader may refer to [2] where it is shown that $\overline{\boldsymbol{T}}$ reflects material texture and irregularities in grain shape and in layer thickness. At last, the two tensor $\boldsymbol{D}$ and $\overline{\boldsymbol{D}}$ stand as damage parameters testifying about degradation mechanism generated within the aggregate. Since no sliding is allowed for closed defects (infinite friction coefficient), these defects do not contribute to the degradation of material (as shown by the summations over layers $\beta\in L^{open}$ in $(3)_{2,3}$). The tensorial parameters $\boldsymbol{D}$ and $\overline{\boldsymbol{D}}$ - in addition to the textural tensor $\overline{\boldsymbol{T}}$ related to initial morphology - allow to account, in a general 3D context, for coupling of primary anisotropy (of any) with the damage-induced one. Note that $\boldsymbol{D}$ and $\overline{\boldsymbol{D}}$ account also for the granular character of the microstructure through the vectors $\boldsymbol{d}^{\beta}$ involved in their definition. As an illustration, the form of the strain $\boldsymbol{\varepsilon}^{\alpha}$ for any layer α (debonded or not) is given below:

$$\boldsymbol{\varepsilon}^{\alpha}=\overbrace{\boldsymbol{C}^{\alpha}\left(\overline{\boldsymbol{T}},\boldsymbol{D},\overline{\boldsymbol{D}}\right):\boldsymbol{E}}^{\varepsilon^{\alpha(r)}} +\varepsilon^{\alpha(d)}\left(\left\{\boldsymbol{\varepsilon}^{\beta D}\right\},\left\{\boldsymbol{\varepsilon}^{fD}\right\};\overline{\boldsymbol{T}},\boldsymbol{D},\overline{\boldsymbol{D}}\right) +\begin{cases}\varepsilon^{\alpha D} & \text{if layer } \alpha \text{ is debonded}\\ \varnothing & \text{if not}\end{cases} \qquad (4)$$

Three contributions are put forward in (4). The first one, $\boldsymbol{\varepsilon}^{\alpha(r)}$, is reversible with respect to $\boldsymbol{E}$ (with $\boldsymbol{C}^{\alpha}$ the corresponding strain localisation tensor degraded, via $\boldsymbol{D}$ and $\overline{\boldsymbol{D}}$, by the presence of open defects inside the volume). The second one, $\boldsymbol{\varepsilon}^{\alpha(d)}$, involve the full set $\{\boldsymbol{\varepsilon}^{\beta D}\}\cup\{\boldsymbol{\varepsilon}^{fD}\}$ related to the effect of any kind of defects (open and closed) in the material. The last one, $\boldsymbol{\varepsilon}^{\alpha D}$, corresponds to the contribution of the defects (if any) located at the interfaces of the considered layer α.

Due to infinite friction, $\boldsymbol{\varepsilon}^{fD}$, for a layer $f\in L^{closed}$ with closed defects at its interfaces, does not depend on the macroscopic strain $\boldsymbol{E}$ since no sliding is allowed. As a result, the set $\{\boldsymbol{\varepsilon}^{fD}\}$ acquire the status of internal variables accounting for the distortion due to the blockage of closed defects inside the volume. On the contrary the opening of a defect naturally depends on $\boldsymbol{E}$ and therefore $\boldsymbol{\varepsilon}^{\beta D}$ also. Indeed, it is recalled that $\boldsymbol{\varepsilon}^{\beta D}$ represents, for a layer $\beta\in L^{open}$, the contribution to its total strain of the open defects located at its own interfaces. The foregoing scale transition is then completed by a second stage –called complementary localization-homogenization procedure in [1] - in order to establish the explicit dependence of $\boldsymbol{\varepsilon}^{\beta D}$ on global strain $\boldsymbol{E}$. Using thermodynamics as a guide, the mean advantage of such an approach is its possible generalization for time-dependant materials. In elasticity, the strain $\boldsymbol{\varepsilon}^{\beta D}$ induced in a layer β by the open defects at its own interfaces, is obtained as a function of $\boldsymbol{E}$, $\boldsymbol{D}$, $\overline{\boldsymbol{D}}$ and local morphological features as follows:

$$\varepsilon_{ij}^{\beta D} = -Id_{ijmu} d_v^\beta n_m^\beta / h^\beta M_{uvkl} E_{lk} + r_{ij}^{\beta D} \quad (5)$$

The detailed form for $\boldsymbol{M}(\overline{\boldsymbol{T}}, \boldsymbol{D}, \overline{\boldsymbol{D}})$ is given in [1]. The constant tensor $\boldsymbol{r}^{\beta D}$ with respect to $\boldsymbol{E}$, represents a residual strain induced in the layer β by residual opening of the defects at its interfaces after global unloading (*i.e.* $\boldsymbol{E} = \boldsymbol{0}$). Physically, such a residual opening is likely linked to the roughness of corresponding interfaces. With (5), local strain field and global response of the elastic damaged composite, are expressed in terms of global strain $\boldsymbol{E}$, distortion internal variables $\{\boldsymbol{\varepsilon}^{fD}\}$, residual opening strain-like quantities $\{\boldsymbol{r}^{\beta D}\}$, and damage tensorial parameters $\boldsymbol{D}$ and $\overline{\boldsymbol{D}}$ testifying about deterioration.

3 Damage state and configuration evolution, discrete modeling

Thanks to its explicit schematization of the real microstructure notably of the grain/matrix interfaces in addition to the accessibility to an estimate of local fields, the MA allows to treat damage evolution at the local scale, that of the constituents. Thus, instead of considering $\boldsymbol{D}$ and $\overline{\boldsymbol{D}}$ as macroscopic damage internal variables and establishing evolution equations for these variables, the direct discrete modeling is put forward here considering the sequence of discrete interfacial local damage events. In such a strategy $\boldsymbol{D}$ and $\overline{\boldsymbol{D}}$ remain as damage parameters reflecting induced degradation and anisotropy in the local and global estimates. Two criteria are thus formulated exploiting the morphological characterization of the interfaces and the knowledge of the displacement field expression due to the kinematical assumptions posed at the very basis of the MA. The first one concerns the nucleation of new defects, and the second one is a closure criterion, which allows to describe the evolution of damage configuration (*i.e.* the respective proportion of open and closed defects for a given total number of defects). Practically, the both criteria will be tested for each increment of a simulated loading path. When one criterion will be satisfied for one or several interfaces, the parameters $\boldsymbol{D}$ and $\overline{\boldsymbol{D}}$ will be actualized in consequence (by adding or suppressing elements in the summations, see $(3)_{2,3}$).

3.1 Nucleation criterion

Following the hypothesis of no sliding ('infinite friction coefficient'), the nucleation is supposed to happen in a mode I fashion.

Consider a layer α with sound interfaces. The displacement field in this layer is noted $\boldsymbol{u}^\alpha$, and it is noted $\boldsymbol{u}^0$ in the grains. Two particular points P_1 and P_2 are then defined on each side of the first interface I_1^α, the one in the grain and the other in the matrix. Both points are equidistant from their normal projection B_1 on the interface, with B_1 the gravity center of I_1^α (see Fig.2).

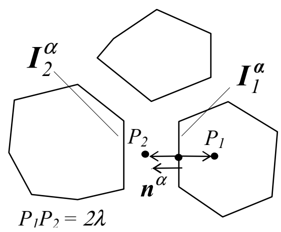


Fig. 2. Definition of testing points P_1 and P_2.

The difference $\Delta\boldsymbol{u}=\boldsymbol{u}^\alpha(P_2)-\boldsymbol{u}^0(P_1)$ is expressed using the linearity of the fields $\boldsymbol{u}^\alpha$ and $\boldsymbol{u}^0$ (according to the kinematical assumptions Section 2) and the expressions (1) for $\boldsymbol{f}^\alpha$. The knowledge of $\Delta\boldsymbol{u}$ allows to evaluate the normal projection of the difference of actual positions of P_1 and P_2 It is considered that when this distance, noted d^α_{norm}, reaches a certain critical value, decohesion happens at the interfaces of the layer α:

$$d^\alpha_{norm} = d_{critical} \Leftrightarrow \text{debonding} \quad (6)$$

$$d^\alpha_{norm} = 2\lambda + \Delta\boldsymbol{u} \bullet \boldsymbol{n}^\alpha$$

It is stressed that d^α_{norm} depends (via $\Delta\boldsymbol{u}$) on morphological parameters of the layer α and on damage configuration if any other layer is already debonded in the volume (see [12] for detailed form of $\Delta\boldsymbol{u}$).The value $d_{critical}$ is a sort of critical defect-incipience opening, depending on the material studied and linked to the

adhesion properties of the matrix on the grains. Moreover, it is to be noted that the identification of $d_{critical}$ for a particular composite will depend on the characteristic length 2λ (distance chosen between two points P_1 and P_2 on each side of the interface).
Since decohesion is supposed to take place in a primarily normal mode, a layer α for which (6) is satisfied becomes a layer of type β (namely with open defects at its interfaces). The contribution to its strain of the defects at stake is then given by (5). The summations involved in the definition of the parameters $\boldsymbol{D}$ and $\overline{\boldsymbol{D}}$ are actualized by adding this new layer.

3.2 Closure criterion

The closure criterion is given in terms of local normal displacement jump in the following way for a layer β with open defects at its interfaces:

While $\langle \boldsymbol{b} \rangle_{I_1^\beta} \bullet \boldsymbol{n}^\beta > 0$ defects at the interfaces of the layer β are open

When $\langle \boldsymbol{b} \rangle_{I_1^\beta} \bullet \boldsymbol{n}^\beta = 0$ defects at the interfaces of the layer β are closed

The test of the closure criterion requires the calculation of the average displacement jump. Considering the affine form of the jump across the interface I_1^β, the latter is linked to $\boldsymbol{f}^{\beta D}$ via: $\langle \boldsymbol{b} \rangle_{I_1^\beta} = \boldsymbol{f}^{\beta D} \boldsymbol{y}^{B_1}$ with $\boldsymbol{y}^{B_1}$ the coordinates of B_1. The symmetric part of $\boldsymbol{f}^{\beta D}$, $\boldsymbol{\varepsilon}^{\beta D}$, is known via (5). The determination of the rotation $\boldsymbol{\omega}^{\beta D}$ makes use of a specific treatment. The key concept is to search the rotation axis of the layer β precisely when its interfaces get debonded. This axis is searched as the edge of the interface I_1^β for which the difference of displacement vectors of two points on each side of this edge is minimum. A local basis is thus defined at the nucleation and conserved further. The rotation tensor $\boldsymbol{\omega}^{\beta D}$ is calculated at each loading step using this basis and so that the mean displacement jumps on both interfaces be opposite. By this way, $\boldsymbol{f}^{\beta D}$ and therefore the mean displacement jump may be evaluated and the closure criterion performed at each loading step.

When the closure criterion is satisfied, the layer β becomes a layer of type f (namely with closed defects at its interfaces). The contribution, $\boldsymbol{\varepsilon}^{fD}$, to its strain of the closed defects is then obtained using (5) at defect closure:

$$\boldsymbol{\varepsilon}^{fD} = \boldsymbol{\varepsilon}^{\beta D}(\boldsymbol{E}_{closure\beta}) \qquad (7)$$

with $\boldsymbol{E}_{closure\beta}$ the corresponding global strain tensor. Then, the summations involved in the definition of the parameters $\boldsymbol{D}$ and $\overline{\boldsymbol{D}}$ are actualized by suppressing one element. Due to the infinite friction coefficient, $\boldsymbol{\varepsilon}^{fD}$ does not evolve as long as the defects remain closed.

4 Numerical illustration

A discrete numerical solving procedure to estimate via the MA the local and global responses of a material under a loading generating damage has been coded in Fortran 90. As an illustration of its applicability and qualitative relevance, the results obtained in the case of successive or simultaneous discrete interfacial events (nucleation and closure of defects) occurring in a specific three-dimensional random composite are presented.

4.1 Material description and loading path

The composite studied is constituted of 400 polyhedral grains embedded in a matrix occupying 25 per cent of the total volume. Such a microstructure has been numerically generated in order to respect the requirements of the geometrical schematization (polyhedral grains, plane and parallel opposite interfaces…) and the compatibility condition briefly mentioned in subsection 2.2. The morphological parameters h^α, A^α, $\boldsymbol{n}^\alpha$ and $\boldsymbol{d}^\alpha$ (see subsection 2.1) have been identified by simple geometrical measures for each of the *2400* layers present in the microstructure. Elastic moduli of the constituents are as follows: $E = 120GPa$, $\nu = 0{,}3$ for the grains and $E = 4$GPa, $\nu = 0{,}45$ for the matrix. Evidently, these values are not those of propellant materials. They are chosen in order to stay in the small strain framework at the local level. In the same way, the critical value, $d_{critical}$, is tentatively chosen as follows: $d_{critical} = 3{,}548\ \mu m$ and $\lambda = h/10$ where $h=0{,}029mm$ is the thickness of the thinnest layer in the volume. At last, the roughness of interfaces is here neglected and therefore strain-like quantities $\boldsymbol{r}^{\beta D}$ are taken as nulls.

The macroscopic displacement gradient $\boldsymbol{F}$ (and corresponding $\boldsymbol{E}$) are the only data required by the MA to define the loading path; indeed no boundary conditions have to be explicitly posed on the volume boundaries. The composite is subjected to the following incremental loading path:

1/ "Tension": incremental extension in the direction ***1*** ($\Delta F_{11}>0$) whereas contractions are applied in directions **2** and **3** with $\Delta F_{22} = \Delta F_{33} = -0{,}3\ \Delta F_{11}$;

2/ Simple shear: $\Delta F_{12} > 0$;

3/ "Compression": incremental loading inverse to the first one (contraction in the direction ***1*** with $\Delta F_{11} < 0$ and extensions in directions ***2*** and ***3*** with $\Delta F_{22} = \Delta F_{33} = -0{,}3\ \Delta F_{11}$).

4.2 Homogenized stress as a function of damage local events

Since all the interfaces are characterized and the criteria formulated at the scale of these interfaces, the AM gives access to the position and morphology of defects within the microstructure in addition to the homogenized response. These results allow the construction of 3D representations of the damaged microstructure. Since the nucleation has been supposed in normal mode, a defect is open before being closed. In order to clearly detect the opening/closure transitions, only open defects are represented in the visualizations. When open defects are nucleated they appear and when they close they disappear. Obviously, it does not mean that closed defects are no longer present in the microstructure.

Fig.3 presents the evolution of the homogenized stress Σ_{11} with macroscopic axial strain E_{11}. For significant points ((1) to (9)) in Fig. 3, Fig. 4 presents 3D visualisations of the microstructure, showing the position and orientation of open defects, and also representations of the homogenized Young's modulus in the plane *(1,2)*, *i.e.* $E(\mathbf{m})$, with **m** arbitrary direction of the plane. These latter representations allow to follow the evolution of damage induced anisotropy (embodied by the tensorial parameters $\boldsymbol{D}$ and $\overline{\boldsymbol{D}}$). Parallel setting of Fig. 3 and 4 allows the following observations:

- (1): sound material, elastic linear behavior
- From (2) to (4): progressive nucleation of defects (red) with normal close to ***1*** as expected with a nucleation criterion in normal mode considering the loading in the direction ***1***. The response is non linear with progressive softening. At the end of «tension», E is principally degraded in the axial direction ***1***.
- Between (4) and (5): the simple shear leads to the nucleation of defects (green) with normal more dispersed. These defects add to the first population. The parameters $\boldsymbol{D}$ and $\overline{\boldsymbol{D}}$ evolve, Σ_{11} decreases whereas E_{11} is constant. At the end (5), the anisotropy is more pronounced, see the ellipsoidal form of $E(\mathbf{m})$.
- After (5), the «compression» begins. A first stage before the truly «compression» $E_{11} < 0$ consists in the unloading of E_{11} until $E_{11} = 0$. In the zoomed zone (green in Fig. 3) one may observe the progressive closure of defects, in particular those nucleated in «tension» which are all closed in (7). This leads to the progressive recovery of E (via suppression of elements in $\boldsymbol{D}$ and $\overline{\boldsymbol{D}}$). The recovery is complete when the (green) defects nucleated during simple shear are also closed (8). These results illustrate the ability of the MA to deal with unilateral effects. At last, one observes residual macroscopic effects (see Fig. 3) due to the distorsion of closed defects (through $\{\boldsymbol{\varepsilon}^{fD}\}$).
- When pursuing the «compression», defects normal to transverse directions ***2*** and ***3*** are nucleated. At the end, E is degraded in the direction ***2*** as illustrated Fig. 4, but not in the axial direction since the closed defects are blocked due to infinite friction coefficient.

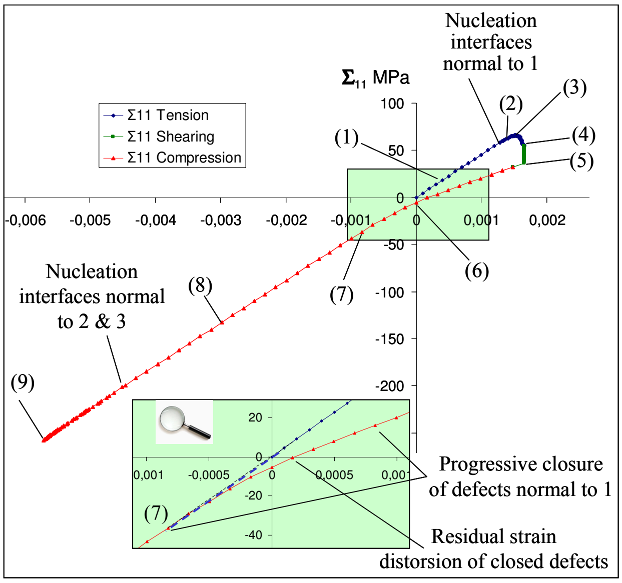
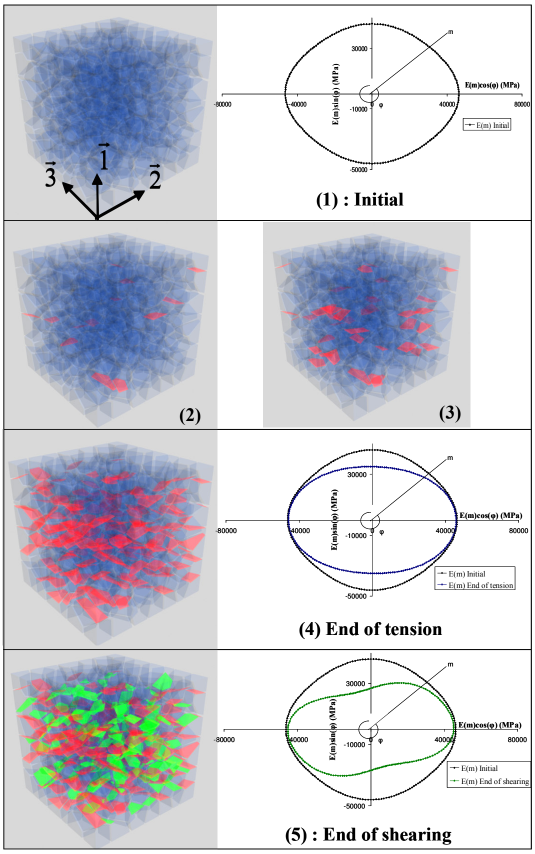


Fig.3. Homogenized Σ_{11} versus E_{11} for simulated “tension” - simple shear - “compression”



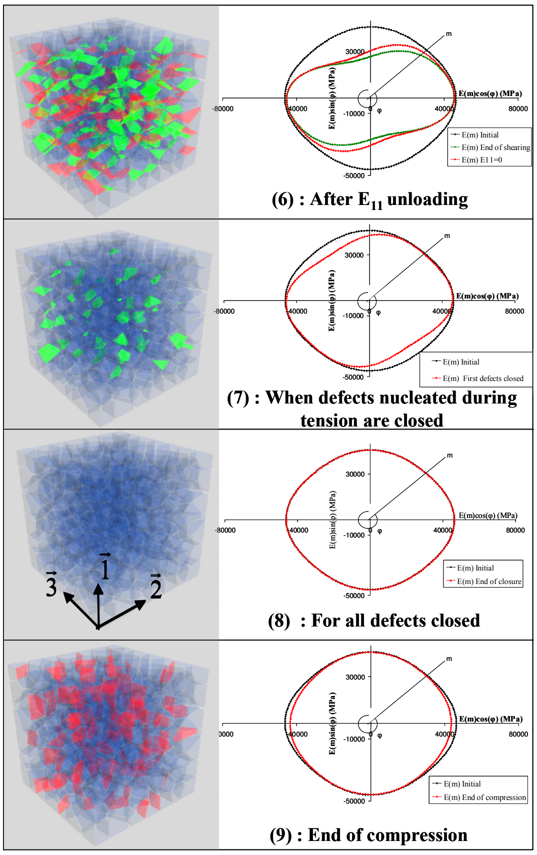


Fig.4. Damaged microstructure and corresponding macroscopic induced anisotropy for simulated “tension” - simple shear - “compression”

4 Conclusion and prospects

The MA stands as a *direct* scale transition approach for modeling the non linear behavior of highly-filled particulate composites. Its direct character is manifest through several aspects. First, the MA starts by a *direct* geometrical schematization of the real microstructure. Second, one may notice the *direct* character of the solving procedure of the localization-homogenization problem. Indeed, most of existing non linear homogenization schemes are referring to the notion of equivalent linear composite and need prior linearization of the non linear constitutive behavior. This linearization procedure may have a strong influence on the global estimates (see *e.g.* [11]) and make difficult the introduction of damage. For the MA, the non linear constitutive laws do not need any prior modification. Moreover, as shown by [3], the MA solving procedure for viscoelastic composites regards directly the time-domain contrarily to most of current approaches using the correspondence principle and the Laplace-Carson transform. This is once again an advantage for the description of damage. At last, one may emphasize the direct accessibility to an estimate of local fields (everywhere except around grain edges) and this, in a non linear context.

The above specificities are due to both direct geometrical schematization and associated simplified kinematical description constituting the very basis of the MA. These two ingredients make the MA *direct* as recalled before and therefore relevant to deal with damage. Thanks to its direct characterization of all the interfaces in addition to the accessibility to local fields, the MA allows to treat damage evolution as a discrete sequence of interfacial events (nucleation and/or closure of defects). Two local criteria have been proposed to this aim. As illustrated by the simulation performed in the preliminary framework of linear elastic constituents (Section 4), the MA is able to provide the evolution of the estimated homogenized response, notably its anisotropy, as a function of the chronology of local damage events whose characteristics are accessible (position and morphology of defects) as required by the application context. Moreover, the results obtained seem to confirm the relevance of the kinematical description, already observed by [6] for undamaged materials, and that of the additional assumptions advanced for the damage modeling itself. At last, CPU time required for a simulation is very low (less than 10mn for the loading path studied with a processor Pentium 4). Nevertheless, a limit due to the kinematical description lies in the impossibility to deal with partial debonding.

According to the application context, the MA is devoted to propellant-like materials. The results obtained for sound viscohyperelastic composites by [6,10] as well as those here obtained in elasticity in the presence of damage allows us to be optimist regarding the ability of the MA to provide essential data required by reactive models. To this end, the MA has to be however extended to deal with both finite strain non linear local behaviors and damage. At last, it is stressed that the accuracy of the MA estimates regarding location and morphology of defects within a real propellant will be strongly influenced by the quality of the polyhedrization. Special investigations are under way in order to optimize this crucial stage.

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