

Modelling the onset and propagation of damage of matrix/inclusion type heterogeneous media with differential swelling

Vincent Gauthier, Renaud Masson, Mihail Gãrãjeu, Bruno Michel, Thomas

Helfer

▶ To cite this version:

Vincent Gauthier, Renaud Masson, Mihail Gãrãjeu, Bruno Michel, Thomas Helfer. Modelling the onset and propagation of damage of matrix/inclusion type heterogeneous media with differential swelling. CFM 2022 - 25ème Congrès français de mécanique, AFM (Association Française de Mécanique), Aug 2022, Nantes, France. cea-03954985

HAL Id: cea-03954985 https://cea.hal.science/cea-03954985

Submitted on 24 Jan 2023 $\,$

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers. L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Modelling the onset and propagation of damage of matrix/inclusion type heterogeneous media with differential swelling.

V.Gauthier^a, R.Masson^a, M.Garajeu^b, B.Michel^a, T.Helfer^a

a. CEA, IRESNE, DEC, SESC, Cadarache, 13108 Saint Paul Lez Durance, France b. Aix-Marseille Univ, CNRS, Centrale Marseille, LMA, F-13453 Marseille, France

Résumé

Ces travaux visent à étudier le comportement effectif d'un matériau composite de type matrice inclusions, libre de contraintes sur sa surface extérieure et dont les inclusions sont soumises à un gonflement différentiel isotrope monotone. La matrice de ce composite est élastique fragile. Les conditions d'apparition de l'endommagement (phase d'amorçage) sont tout d'abord étudiées, ce qui conduit à la proposition d'un critère, fondé sur un bilan d'énergie, dépendant de la taille et de la fraction volumique des inclusions ainsi que de l'énergie à rupture de la matrice. Pour une dilatation évoluant de façon monotone avec le temps, nous étudions l'amorçage et la propagation de l'endommagement en nous appuyant sur une formulation variationnelle de type champ de phase et en utilisant dans ce cadre une approximation « champ moyen ». La longueur caractéristique du modèle champ de phase est choisie en cohérence avec le critère d'amorçage défini auparavant. L'approximation champ moyen permet ainsi de construire une borne supérieure dont les prédictions sont comparées à des résultats de calculs à champ complet.

Abstract :

This work aims at studying the effective behavior of a particulate composite material (matrix -inclusions type). The composite is stress free at its outer boundary but the inclusions are subjected to a monotonically increasing isotropic differential swelling. The matrix of this composite is brittle elastic. The onset of the damage of the matrix is first studied, which leads to the proposal of a criterion based on an energy balance, depending on the size and the volume fraction of the inclusions as well as the fracture energy of the matrix. For a dilatation increasing monotonously with time, we study the onset and the propagation of the damage by relying on a variational formulation (phase field approach) and by using in this framework a "mean field" approximation. The characteristic length of the phase field model is chosen accordingly to the onset of damage criterion defined previously. An upper bound is then constructed and its predictions are compared to the results of full field calculations.

Mots clefs : Two-phases composite, Swelling, Brittle behavior, Phase field, Variational principle, Hashin-Shtrikman bound.

1 Introduction

Many works have already been carried out to model and study the damage of structures. Several approaches have been proposed, such as the linear fracture mechanics or the damage mechanics.

In parallel, in order to yield the effective behavior of a heterogeneous material, meaning taking into account the microstructural properties of the material, two complementary approaches may be followed. On the one hand, it is possible to perform full field computations that consist in running numerical simulations based mainly either on the finite element ([1, 2]) or on the FFT method ([3]). Computation of the average of the mechanical fields over the volume gives the effective behavior. On the other hand, rather than performing numerical computations, it may be preferred to carry out a semi-analytical analysis to derive the effective behavior. Those approaches are referred to as mean field computations methods and encompass the homogenization techniques that establish estimations of the effective behavior, for instance the well-known Mori-Tanaka scheme [4] or the Hashin-Shtrikman bounds [5] in the case of an elastic behavior. A huge literature exists on that subject.

This work seeks to determine the effective behavior of a two phases matrix/inclusions composite with a brittle matrix and a swelling prescribed to the inclusions. For that loading, a micromechanical approach is required to study the whole stress relaxation process. In contrast with the work realized in [6], where the stress relaxation comes from a viscous behavior, in the present case the damage is the only source of stress relaxation.

The article is divided into three parts. The first part is devoted to the description of the studied mechanical problem as well as the phase field approach ([7, 8]) adopted to model the damage evolution.

The second part is focused on the definition of the onset of damage in the considered two-phase matrixinclusions microstructure submitted to a differential dilatation. A methodology, based on an energy balance over the matrix, is then proposed to estimate the loading conditions that must be met to satisfy the damage onset criterion.

In a third part, we conjugate the variational principle attached to the phase field approach with mean field homogenization techniques to yield estimates of the effective behavior.

2 The mechanical problem

In this work we consider a two phases microstructure occupying a domain V, made up of an inclusion phase, denoted (2) and a matrix, denoted (1). Both have the same young modulus E = 200 GPa and the same Poisson ratio $\nu = 0, 3$ (κ and μ denote the bulk and shear moduli in the sequel while the fourth-order tensor of moduli is denoted by C). The inclusions are subjected to an isotropic monotonic increasing swelling $\varepsilon_0^{(2)} = \varepsilon_0^{(2)} \delta$ (δ the identity for the symmetric second-order tensors) which generates an heterogeneity inside the microstructure. In addition, the boundary of the composite is stress free $\bar{\sigma} = 0$ where $\bar{\sigma}$ denotes the macroscopic stress.

The matrix is the phase that displays a brittle elastic behavior. Thus, its critical energy release rate is the following $G_c = 1 J/m^2$ [9]. For a later use, the volume fraction of each phase is denoted by $c^{(j)}$ (hereafter, $c^{(2)} = 18\%$), the mean radius of the inclusions is denoted by a (hereafter, $a = 30 \mu m$)

and the volume average of a quantity over the volume $V^{(j)}$ occupied by the phase (j) is denoted by $\overline{q}^{(j)} = \langle q \rangle^{(j)} = \frac{1}{V^{(j)}} \int_{V^{(j)}} q \, dx$, with $j \in 1; 2$.

2.1 Phase field model

This work makes use of a phase field approach for damage whose principle was first introduced in [7] and consists in minimizing the potential energy of a structure. For implementation on numerical codes, regularizations have been later proposed, in [8]. More details about this regularization may be found in [10, 11]. The main feature of those models is the replacement of the crack surface by a smooth scalar field, called the phase field, and denoted d.

For further developments, one defines the sets of admissible fields for a given instant t_n :

$$V_n = \{ \boldsymbol{u}^*(t_n) \in \boldsymbol{H}^1, \boldsymbol{u}^*(t_n) = \boldsymbol{u}_n \text{ on } \partial V_d \}$$

$$D_n = \{ d^*(t_n) \in \boldsymbol{H}^1, d^*(t_n) \ge d(t_{n-1}), \text{ in } V \}$$
(1)

where H^1 is a Sobolev space, ∂V_d is the fraction of the boundary where a displacement is prescribed. In addition $d^*(t_n) : V \to [0, 1]$. It is noteworthy that the two fields u^* and d^* depend on the spatial variable x which is omitted here. Similarly, the time dependency of those two fields is omitted in next expressions, for convenience.

The problem to solve is the following :

$$\min_{(\boldsymbol{u}^*, d^*) \in (V_n \times D_n)} W(\boldsymbol{\varepsilon}_0^{(2)}, \, \boldsymbol{\varepsilon}(\boldsymbol{u}^*), d^*)$$
(2)

with the functional W defined by the relation :

$$W(\boldsymbol{\varepsilon}_{0}^{(2)}, \, \boldsymbol{\varepsilon}(\boldsymbol{u}^{*}), d^{*}) = \frac{1}{2} \int_{V} \chi^{(1)}(\boldsymbol{x}) \left[g(d^{*}) \boldsymbol{\varepsilon}(\boldsymbol{u}^{*}) : \boldsymbol{C} : \boldsymbol{\varepsilon}(\boldsymbol{u}^{*}) \right] d\boldsymbol{x} + \int_{V} \chi^{(1)}(\boldsymbol{x}) \left[\frac{G_{c}}{c_{w}} \left(\frac{\Theta(d^{*})}{l_{c}} + l_{c} \nabla d^{*} \nabla d^{*} \right) \right] d\boldsymbol{x}$$
(3)
$$+ \frac{1}{2} \int_{V} \chi^{(2)}(\boldsymbol{x}) \left(\boldsymbol{\varepsilon}(\boldsymbol{u}^{*}) - \boldsymbol{\varepsilon}_{0}^{(2)} \right) : \boldsymbol{C} : \left(\boldsymbol{\varepsilon}(\boldsymbol{u}^{*}) - \boldsymbol{\varepsilon}_{0}^{(2)} \right) d\boldsymbol{x}$$

(with $\chi^{(j)}$ the characteristic function of phase $j = 1, 2 : \chi^{(j)}(x) = 1$ if $x \in V^{(j)}$, zero otherwise). In this work, the choice is made to make use of the Ambrosio-Tortorelli 2 [10] model :

$$\begin{cases} g(d^*) = (1 - d^* + k_c)^2 \\ \Theta(d^*) = d^{*2} \\ c_w = 2 \end{cases}$$
(4)

The solutions of the problem (2) are denoted (u, d).

In the expression of the phase field model, three parameters are introduced : the critical energy release rate G_c (already defined as a matrix property above), the characteristic length l_c and the k_c parameter. The characteristic length corresponds to the thickness of the process zone and can be assigned either a material [12, 9] (related to the failure stress) or a regularization (related to the Griffith case) definition. In parallel, the k_c parameters corresponds to the residual stiffness of a totally damaged element, in order to make the convergence easier.

An implementation making use of a staggered scheme under the finite element software CAST3M have been proposed in [13, 14] and was further adapted in [9] for the case of the composite studied in this article and will be further developed in section 4.3.

2.2 Expected effective behavior

Due to the swelling prescribed to the inclusions, the matrix experiences tensile stresses while the inclusions are under compression. For low values of this swelling, the matrix remains elastic. As the elastic moduli are uniform, the overall macroscopic strain is simply given by the volume average of the swelling, namely : $\overline{\epsilon}(t) = c^{(2)} \varepsilon_0^{(2)}(t) \delta$.

Conversely, when the matrix phase is fully damaged, the stress field in the matrix phase vanishes, namely :

$$\forall \boldsymbol{x} \in V^{(1)} \quad \boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{0} \tag{5}$$

In fact, the nil stress field $\boldsymbol{\sigma} = \mathbf{0}$ and the homogeneous displacement field $\boldsymbol{u}(\boldsymbol{x}) = \varepsilon_0^{(2)} \cdot \boldsymbol{x}$ are respectively statically admissible and kinematically admissible. In addition, they satisfy the constitutive laws :

- in the inclusions : $\boldsymbol{\sigma} = \mathbf{0} = \boldsymbol{C}^{(2)} : (\boldsymbol{\varepsilon} \boldsymbol{\varepsilon}_0^{(2)}) = \mathbf{0}$
- and in the fully damaged matrix : $\sigma = 0$.

As a result, these particular admissible fields :

$$\boldsymbol{x} \in V \quad \boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{0} \quad \text{and} \quad \boldsymbol{u}(\boldsymbol{x}) = \varepsilon_0^{(2)} \cdot \boldsymbol{x}$$

are solutions so that the macroscopic strain in the fully damaged regime reads : $\bar{\varepsilon}_m = \varepsilon_0^{(2)}$

3 Definition of the onset of damage

In [1], a dispersion of pressurized voids in a ceramic matrix was considered. In order to describe properly the onset of damage, the geometry of the bubbles had first to be defined; each bubble featuring a defect. Then, thanks to a Griffith criterion (making use of the energy release rate G), the critical pressure p_c to prescribe to the bubbles was given, with the relation :

$$G_{\theta}(p_c) = G_c \tag{6}$$

It was then possible to determine the failure stress by approximating the bubble geometry by a sphere. The critical stress was given by the hoop stress on its periphery which is equal to $\frac{p_c}{2}$. Although this approach is appealing, it is not completely suitable for this study since numerical computations are required to determine G. In addition, the shape of the defect remains arbitrary. This is the reason why it is chosen to simplify the problem in order to dispose of a problem that can be solved analytically.

The simplification must take into account that the onset of damage appears in the vicinity of each inclusion, each inclusion being considered isolated but in interaction with the surrounding matrix. This is why the composite sphere structure is kept, where a matrix phase, with a radius denoted by *b* embeds an inclusion phase with the radius *a*; the radii being related to the volume fraction $c^{(2)}$ of the inclusions phase with the expression : $b = a (c^{(2)})^{-1/3}$. Furthermore, the defect, initially present in [1], is removed in this situation and replaced by the final crack surface (matrix totally broken in one of its hemispheric plane). The situation is depicted in figure 1.



FIGURE 1 – Situation considered for the sphere composite criterion, the red line embodies the crack surface around the inclusion [9]

Finally, an energy balance inspired from the Griffith criterion [9] is proposed :

$$\left(U_{el} - 2U_{el}^{h}\right) \frac{4\pi}{3} \left(b^{3} - a^{3}\right) = G_{c} \pi \left(b^{2} - a^{2}\right)$$
(7)

 U_{el} being the density of elastic energy stored in the matrix phase at the onset of fracture while U_{el}^h denotes the same quantity stored in each part of the composite sphere, once separated by the crack. This last term will be neglected in the sequel $U_{el}^h \approx 0$. However, the left-hand term of equation (7) can be easily computed as the displacement field respects the spherical symmetry in that particular situation, namely :

$$\frac{4\pi}{3} (b^3 - a^3) U_{el} = \frac{24\pi\kappa_e \,\mu_e(\varepsilon_g^{(2)})^2}{(3\kappa_e + 4\mu_e)^2} \, a^3 c^{(1)} (4\mu_e c^{(2)} + 3\kappa_e) \tag{8}$$

Injecting the expression (8) into the energy balance (7), the critical value of the loading $\varepsilon_{0c}^{(2)}$ is the following :

$$\varepsilon_{0c}^{(2)} = \sqrt{\frac{G_c}{a} \frac{(3\kappa + 4\mu)^2}{24\kappa\mu (4\mu c^{(2)} + 3\kappa)} \frac{(1 - (c^{(2)})^{\frac{2}{3}})}{c^{(1)} (c^{(2)})^{\frac{2}{3}}}}$$
(9)

In conclusion, the onset of damage criterion yields a value for the critical swelling to prescribe which depends only on microstructural parameters like the mean size of the inclusions and their volume fraction, the elastic moduli of both phases as well as the critical energy release rate G_c of the matrix phase. For the considered data, the critical loading is $\varepsilon_{0c}^{(2)} = 5,76 \times 10^{-4}$.

4 Mean field estimate of the damage propagation

The goal of this section is to take advantage of the variational principle (2) from which phase field equations are derived to establish an upper bound for the elastic energy of the damaged microstructure. The corresponding effective behavior will then be estimated with linear homogenization schemes, and

in particular the upper bound of Hashin-Shtrikman.

4.1 An upper bound derived from the variational principle (2)

First of all, a macroscopic strain $\bar{\varepsilon}$ is prescribed to the outer surface of $V (\partial V_d = \partial V \text{ in } (1))$ so that this macroscopic strain loading appears explicitly in the expression of the functional W denoted hereafter by $W(\bar{\varepsilon}, \varepsilon_0^{(2)}, \varepsilon(u^*), d^*)$. In addition, it is more convenient for next developments to rewrite the functional (3) in the following way :

$$W(\bar{\boldsymbol{\varepsilon}}, \, \boldsymbol{\varepsilon}_0^{(2)}, \, \boldsymbol{\varepsilon}(\boldsymbol{u}^*), \, d^*) = \int_V w_{FM}(\boldsymbol{\varepsilon}_0^{(2)}, \boldsymbol{\varepsilon}(\boldsymbol{u}^*), d^*) \, d\,\boldsymbol{x}$$
(10)

where a potential $w_{FM}(\boldsymbol{\varepsilon}_0^{(2)}, \, \boldsymbol{\varepsilon}(\boldsymbol{u}^*), \, d^*)$ has been introduced and is defined by :

$$w_{FM}(\boldsymbol{\varepsilon}_{0}^{(2)}, \, \boldsymbol{\varepsilon}(\boldsymbol{u}^{*}), \, d^{*}) = \chi^{(1)}(\boldsymbol{x})w^{(1)}(\boldsymbol{\varepsilon}(\boldsymbol{u}^{*}), d^{*}) + \chi^{(2)}(\boldsymbol{x})w^{(2)}(\boldsymbol{\varepsilon}(\boldsymbol{u}^{*}), \boldsymbol{\varepsilon}_{0}^{(2)}) \qquad (11)$$
$$+ \chi^{(1)}(\boldsymbol{x}) \left[\frac{G_{c}}{c_{w}} \left(\frac{\Theta(d^{*})}{l_{c}} + l_{c} \nabla d^{*} \nabla d^{*} \right) \right]$$

the strain potentials $(w^{(1)}, w^{(2)})$ being defined by :

$$\begin{cases} w^{(1)}(\boldsymbol{\varepsilon}(\boldsymbol{u}^*), \boldsymbol{d}^*) = \frac{1}{2}g(\boldsymbol{d}^*)\boldsymbol{\varepsilon}(\boldsymbol{u}^*) : \boldsymbol{C} : \boldsymbol{\varepsilon}(\boldsymbol{u}^*) \\ w^{(2)}(\boldsymbol{\varepsilon}(\boldsymbol{u}^*), \boldsymbol{\varepsilon}_0^{(2)}) = \frac{1}{2}\left(\boldsymbol{\varepsilon}(\boldsymbol{u}^*) - \boldsymbol{\varepsilon}_0^{(2)}\right) : \boldsymbol{C} : \left(\boldsymbol{\varepsilon}(\boldsymbol{u}^*) - \boldsymbol{\varepsilon}_0^{(2)}\right) \end{cases}$$
(12)

It is possible to build an upper bound from the expression of the functional (10). The method may be split into two steps. The first steps consists in making assumptions on the form of the damage field in the matrix. The second step consists in the use of the variational principle on which the Francfort-Marigo [7] and the phase field model is based [11, 15]. As a consequence, an inequality will be obtained and studied, thus establishing the upper bound. The two steps are laid out in the rest of the subsection.

As previously told, it is required to make assumptions on the form of the admissible damage field. As a matter of fact, one has to bear in mind that homogenization techniques required a finite number of phases to be able to estimate effective values (average stress, average strain, elastic energy). This cannot be achieved with a damage field that takes an infinite number of values in the interval [0; 1]. The latter amounts to considering an infinite number of phases throughout V. It is possible to diminish the number of phases by assuming that the damage field is uniform over specific areas, likewise the TFA [16] or the NTFA method [17]. This work goes further by assuming that the damage field is uniform *over the matrix phase*.

Thus, the admissible set of damage field is now D'_n defined by :

$$D'_{n} \subset D_{n}$$
 with $D'_{n} = \{ d^{*} \in D_{n} \text{ such as } d^{*}(\boldsymbol{x}, t_{n}) = d^{(1)}(t_{n}), \forall \boldsymbol{x} \in V^{(1)} \}$ (13)

with D_n being the set of admissible damage fields defined in subsection 2.1

In parallel, it is possible to make use of the variational principle introduced in equation (2) with the expression of the functional adapted for this work (10). The admissible fields u^* and d^* that minimize

the functional W being denoted u and d, the minimization process is equivalent to :

$$\forall \boldsymbol{u}^* \in V_n \text{ et } \forall d^* \in D_n, \left\langle w_{FM} \left(\boldsymbol{\varepsilon}_0^{(2)}, \, \boldsymbol{\varepsilon}(\boldsymbol{u}), \, d \right) \right\rangle \leq \left\langle w_{FM} \left(\boldsymbol{\varepsilon}_0^{(2)}, \, \boldsymbol{\varepsilon}(\boldsymbol{u}^*), \, d^* \right) \right\rangle \tag{14}$$

In particular, it is possible to write, for a uniform damage field, considered in this work :

$$\forall \boldsymbol{u}^* \in V_n \text{ et } \forall d^{(1)} \in D'_n, \left\langle w_{FM} \left(\boldsymbol{\varepsilon}_0^{(2)}, \, \boldsymbol{\varepsilon}(\boldsymbol{u}), \, d \right) \right\rangle \leq \left\langle w_{FM} \left(\boldsymbol{\varepsilon}_0^{(2)}, \, \boldsymbol{\varepsilon}(\boldsymbol{u}^*), d^{(1)} \right) \right\rangle$$
(15)

The equation (15) above being true whatever the admissible fields $(u^*, d^{(1)})$, it remains valid in particular :

$$\left\langle w_{FM}(\boldsymbol{\varepsilon}_{0}^{(2)}, \boldsymbol{\varepsilon}(\boldsymbol{u}), d) \right\rangle \leq \min_{d^{(1)} \in D'_{n}} \min_{\boldsymbol{u}^{*} \in V_{n}} \left\langle w_{FM}(\boldsymbol{\varepsilon}_{0}^{(2)}, \boldsymbol{\varepsilon}(\boldsymbol{u}^{*}), d^{(1)}) \right\rangle$$
 (16)

The right term in equation (16) can be re written with the help of equation (11) and remarking that $\nabla d^{(1)} = 0$ as $d^{(1)}$ is homogeneous in the matrix phase :

$$\left\langle w_{FM}\left(\boldsymbol{\varepsilon}_{0}^{(2)},\,\boldsymbol{\varepsilon}(\boldsymbol{u}),\,d\right)\right\rangle \leq \min_{d^{(1)}\in D_{n}^{\prime}}\left[\underbrace{\tilde{W}_{L}(\bar{\boldsymbol{\varepsilon}},\boldsymbol{\varepsilon}_{0}^{(2)},d^{(1)})+c^{(1)}\frac{G_{c}}{c_{w}}\left(\frac{\Theta(d^{(1)})}{l_{c}}\right)}_{\Gamma(\bar{\boldsymbol{\varepsilon}},\boldsymbol{\varepsilon}_{0}^{(2)},d^{(1)})}\right] \tag{17}$$

In (17), one can notice the appearance of the effective elastic energy term \tilde{W}_L of a linear heterogeneous material, referred to as L. The spatial distribution of phases in this linear media is identical to the one of the real microstructure. This linear solid whose phase moduli are $g(d^{(1)}) C$ in the matrix and C in the inclusions respectively, is subjected to the same loading $(\bar{\varepsilon}, \varepsilon_0^{(2)})$. The effective strain energy of this linear elastic material is estimated with the upper bound of Hashin-Shtrikman [5].

If the value of $d^{(1)}$ that minimizes Γ , denoted $\check{d}^{(1)}$, is also a stationary point of Γ , then, the effective behavior corresponding to the upper bound defined in equation (17) is given by the common relation [9]:

$$\bar{\boldsymbol{\varepsilon}} = \tilde{\boldsymbol{S}}_L(\check{d}^{(1)}) : \bar{\boldsymbol{\sigma}} + \tilde{\boldsymbol{\varepsilon}}_0 \tag{18}$$

with \hat{S}_L being the effective compliance of the linear media L and $\tilde{\varepsilon}_0$ its effective (stress-free) swelling (identical to the macroscopic strain when the macroscopic stress vanishes).

4.2 Computation of the mean field solution

Prior the establishment of the effective behavior corresponding to the upper bound, the minimum point of the right hand term of inequation (17) has to be determined. As a matter of fact, the function $\Gamma(\bar{\varepsilon}, \varepsilon_0^{(2)}, d^{(1)})$ is not convex with respect to $d^{(1)}$. That is to say that the number of stationary points within the domain D'_n can be different from one. Moreover, the domain D'_n can be identified with the interval [0; 1] which is compact. So the minimum on [0; 1] may be attained either on the boundary or at a stationary point within]0; 1[, if any. This is why, the first thing to do, is to determine the point where the minimum is reached.

The analytical expression of Γ is the following for the loadings prescribed [9] :

$$\Gamma(\bar{\varepsilon} = \tilde{\varepsilon}_0, \, \varepsilon_0^{(2)}, \, d^{(1)}) = \frac{18c^{(1)}c^{(2)}g(d^{(1)})\,\mu\,\kappa\,\left(\varepsilon_0^{(2)}\right)^2}{\left(3\kappa + 4c^{(1)}\mu\right)g(d^{(1)}) + 4c^{(2)}\mu} + \frac{c^{(1)}G_c}{c_w\,l_c}(d^{(1)})^2 \tag{19}$$

where the constraint $\bar{\varepsilon} = \tilde{\varepsilon}_0$ indicates that the macroscopic strain is chosen such that the macroscopic stress is zero (according to the relation (18) above). The minimum point is then looked for. In figure (2), the procedure is laid out for three loadings in particular.



FIGURE 2 – Graphic representation of $\Gamma(\bar{\epsilon} = \tilde{\epsilon}_0, d^{(1)}, \epsilon_0^{(2)})/D$, with $D = \frac{G_c}{c_w l_c} = 7.32 \times 10^6 \text{ J/m}^3$, versus $d^{(1)}$, for several loadings prescribed : <u>left</u> 1, 07 $\varepsilon_{0c}^{(2)}$; <u>middle</u> 1, 27 $\varepsilon_{0c}^{(2)}$; <u>right</u> : 1, 60 $\varepsilon_{0c}^{(2)}$ [9]

The most particular feature of the function Γ is that there exists a specific swelling prescribed for which there are two points of minimum. This critical behavior is of some importance for the computation of the effective behavior. The graph below underlines the presence of the discrepancy when the prescribed swelling reaches $1,27 \varepsilon_{0c}^{(2)}$. Finally, the effective response of the considered heterogeneous material can



FIGURE 3 – Damage evolution versus the swelling prescribed to the inclusions.

be derived. As the macroscopic stress is zero, the effective response boils down to the determination of the macroscopic strain (identical to the effective stress-free strain in that situation) as a function of the swelling of the inclusions. Denoting the spherical part of the macroscopic strain by $\bar{\varepsilon}_m$, the macroscopic strain is given by the following expression :

$$\begin{cases} \bar{\varepsilon}_m = c^{(2)} B_m^{(2)}(\check{d}^{(1)}) \,\varepsilon_0^{(2)} \\ B_m^{(2)}(\check{d}^{(1)}) = \frac{3\kappa g(\check{d}^{(1)}) + 4\mu}{(3\kappa + 4c^{(1)}\mu)g(\check{d}^{(1)}) + 4c^{(2)}\mu} \end{cases}$$
(20)

where :

— the optimal damage state $\check{d}^{(1)}$ is a function of the swelling (Figure 3).

- $B_m^{(2)}$ denotes the average over phase (2) (inclusions) of the hydrostatic component of the stress localization tensor in the linear composite (L) as estimated by the Hashin-Shtrikman upper bound.

4.3 Comparisons with full-field computations

In [12], the characteristic length l_c is viewed as a material parameter and related to the onset of damage. In this work, this interpretation is preferred over the definition of l_c as a regularization parameter. As a consequence, the choice for l_c to obtain a critical loading consistent with the one defined in the previous section 3 and denoted by $\varepsilon_{0c}^{(2)}$. With this definition, the following value for l_c is obtained : $l_c = 18 \,\mu\text{m}$ (see [9] for details). The k_c parameter has been chosen such that its value does not affect the effective response ($k_c = 10^{-6}$).

For the full-field computations, the RVE size is about $170 \,\mu m$. The inclusions are randomly dispersed within the matrix phase with the RSA algorithm [18]. The minimal distance between the inclusions is $4\mu m$. The RVE has been meshed with about $46 \, 10^4$ linear tetrahedral elements (mesh size $\approx 5 \,\mu m$). More details about these calculations are given in [9]. The effective behavior is plotted in figure (4) versus the prescribed swelling divided by the critical swelling. The following remarks can be made. First,



 $\label{eq:Figure4-Comparison} Figure 4-Comparison between the effective behavior obtained by full field computations and the upper bound.$

a discrepancy exists for a prescribed swelling of $1, 27 \varepsilon_{0c}^{(2)}$ in accordance with the damage jump shown in figure (3). In more physical terms, when the "critical" loading is reached, that the matrix softens suddenly. This discrepancy still needs to be addressed but is probably due the choice of an homogeneous damage field in the matrix and is reminiscent of the unstable propagation of a crack. Extra full field computations with a single inclusion embedded in a matrix may be ran in order to enhance the understanding of the origin of this discrepancy.

Nevertheless, the slope of the graph plotting the macroscopic strain versus the loading prescribed is well described by the upper bound for the elastic behavior, when the loadings prescribed are low $(\dot{\bar{\varepsilon}}_m = c^{(2)} \dot{\varepsilon}_0^{(2)})$. A similar conclusion can be drawn for the case where the matrix is almost totally damaged when higher swellings are prescribed $(\dot{\bar{\varepsilon}}_m \approx \dot{\varepsilon}_0^{(2)})$.

5 Conclusions

The objective of this work was to simulate the damage of a two-phases material (matrix-inclusions microstructure). As the elastic moduli of the two phases are identical, the unique source of heterogeneity is the dilatation prescribed only to the inclusions phase and the damage of the matrix phase. A phase field approach have been adopted to perform these simulations.

The main results are :

- an onset damage criterion is proposed, which gives the conditions that have to be met for the damage to appear in the matrix. The criterion depends only on the microstructural and material parameters.
- by taking advantage of the variational principle attached to the phase field model, an upper bound has been derived.
- this bound sticks well to results derived by full field computations (reported in [9]).
- this upper bound leads to a discontinuous effective behavior.

In order to get rid of the jump of the effective behavior at the transition between the elastic state and the totally damage state, NTFA techniques may be used in the future to introduce a more sophisticated damage fields. In addition, more general loadings should be considered, such as a traction or a shear prescribed to the boundary of the microstructure.

Acknowledgements

This work was developed within the framework of the MISTRAL joint research laboratory between Aix-Marseille University, CNRS, Centrale Marseille and CEA. The authors also acknowledge the financial support of the French Alternative Energies and Atomic Energy Commission (CEA), EDF and FRAMATOME.

Références

- C. Esnoul. <u>Etude du comportement à rupture de la zone HBS du combustible UO2 dans les</u> réacteurs à eau pressurisée, par une approche micromécanique en condition accidentelle d'APRP. PhD thesis, Aix-Marseille Université, 2018.
- [2] M. Seck. Modélisation du comportement effectif de milieux hétérogènes, viscoélastiques, non linéaires et vieillissants; application à la simulation du comportement des combustibles MOX. PhD thesis, Aix-Marseille Université, 2018.
- [3] Y. Chen, D. Vasiukov, L. Gélébart, and C.H. Park. A FFT solver for variational phase-field modeling of brittle fracture. <u>Computer Methods in Applied Mechanics and Engineering</u>, 349 :167–190, 2019.
- [4] T. Mori and K. Tanaka. Average stress in matrix and average elastic energy of materials with misfitting inclusions. Acta metallurgica, 21(5):571–574, 1973.
- [5] Z Hashin and S. Shtrikman. A variationnal approach to the theory of the elastic behaviour of multiphase materials. Journal of Mechanics and Physics of Solids, 11 :127–140, 1963.
- [6] R. Masson, M Seck., J. Fauque, and M. Garajeu. A modified secant formulation to predict the overall behavior of elasto-viscoplastic particulate composites. <u>Journal of Mechanics and Physics</u> <u>of Solids</u>, 137 :103874, 2020.

- [7] G.A. Francfort and J.J. Marigo. Revisiting brittle fracture as an energy minimization problem. Journal of the Mechanics and Physics of Solids, 46(8) :1319–1342, 1998.
- [8] B. Bourdin, G.A. Francfort, and J.J. Marigo. Numerical experiments in revisited brittle fracture. Journal of the Mechanics and Physics of Solids, 48(4) :797–826, 2000.
- [9] V. Gauthier. Modélisation de l'endommagement de microstructures hétérogénes viscoélastiques, application à la simulation du combustible nucléaire MOX. PhD thesis, Aix-Marseille Université, 2021.
- [10] L. De Lorenzis and T. Gerasimov. Numerical implementation of phase-field models of brittle fracture. <u>Modeling in Engineering Using Innovative Numerical Methods for Solids and Fluids</u>, 599 :75–101, 2020.
- [11] B. Bourdin, G.A. Francfort, and J.J. Marigo. The variational approach to fracture. Journal of elasticity, 91(1-3):5–148, 2008.
- [12] H. Amor, J.J. Marigo, and C. Maurini. Regularized formulation of the variational brittle fracture with unilateral contact numercial experiments. <u>Journal of the Mechanics and Physics of Solids</u>, 57 :1209–1229, 2009.
- [13] T. Helfer, B. Bary, T.T. Dang, O. Fandeur, and B. Michel. Modélisation par champ de phase de la fissuration des matériaux fragiles : Aspects numériques et applications au combustible nucléaire oxyde. In <u>13</u>ème colloque national en calcul des structures, 2017.
- [14] Y. Lu, T. Helfer, O. Fandeur, and B. Bary. An efficient and robust staggered algorithm applied to the quasi static description of brittle fracture by a phase field approach. <u>Computer methods in</u> applied mechanics and engineering, 370 :113218, 2020.
- [15] C. Miehe, M. Hofacker, and F. Welschinger. A phase field model for rate-independent crack propagation : Robust algorithmic implementation based on operator splits. <u>Computer Methods in</u> Applied Mechanics and Engineering, 199(45-48) :2765–2778, 2010.
- [16] G.J. Dvorak. Transformation field analysis of inelastic composite materials. <u>Proceedings of the</u> <u>Royal Society of London. Series A : Mathematical and Physical Sciences</u>, 437(1900) :311–327, 1992.
- [17] J.C. Michel and P. Suquet. Nonuniform transformation field analysis. <u>International journal of</u> solids and structures, 40(25) :6937–6955, 2003.
- [18] B. Widom. Random sequential addition of hard spheres to a volume. <u>The Journal of Chemical</u> Physics, 44(10) :3888–3894, 1966.