

An homogenization-based hyperelastic damage model: formulation and application to an EPDM/PP composite

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Abstract

The present Note concerns the formulation, implementation and a first application of a micromechanically based hyperelastic damage model. The approach is based on the second order homogenization method proposed by Lopez-Pamies and Ponte Castañeda (2000) for hyperelastic composites and recently developed by Lopez-Pamies and Ponte Castañeda (2007) in the case of porous elastomers. We first implement the method and proceed to its verification by comparison with Finite Element simulations on a unit cell. Taking advantage of this validation and by using standard thermodynamics arguments, we propose an hyperelastic damage model founded on voids growth phenomena. Finally, we provide an example of validation of the model by comparison with experimental data obtained on an EPDM/PP composite. **To cite this article:** *V. Bouchart et al., C. R. Mecanique 336 (2008)*. © 2008 Académie des sciences. Published by Elsevier Masson SAS. All rights reserved.

Résumé

Un modèle micromécanique d'hyperélasticité avec endommagement : formulation et application à un composite EPDM/PP. La présente Note concerne la formulation, la mise en oeuvre et une application d'un modèle micromécanique d'endommagement dédié aux matériaux hyperélastiques. L'approche suivie repose sur la méthode d'homogénéisation du second ordre proposée par Lopez-Pamies et Ponte Castañeda (2000) pour les composites hyperélastiques et récemment développée par Lopez-Pamies et Ponte Castañeda (2007) dans le cas des élastomères poreux. On met d'abord en oeuvre le modèle dans le cas de milieux poreux et on procède à sa vérification par comparaison à des simulations éléments finis sur une cellule de base. S'appuyant ensuite sur cette validation numérique et utilisant des arguments thermodynamiques standards, on propose un modèle d'endommagement hyperélastique fondé sur des mécanismes de croissance de cavités. Enfin, on fournit un exemple de validation du modèle par comparaison avec des données expérimentales obtenues sur un composite EPDM/PP. **Pour citer cet article :** *V. Bouchart et al., C. R. Mecanique 336 (2008)*.

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Keywords: Damage; Hyperelasticity; Porous materials; Micromechanics; Nonlinear homogenization; Numerical verification; Experimental validation

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Mots-clés : Endommagement ; Hyperélasticité ; Matériaux poreux ; Micromécanique ; Homogénéisation non linéaire ; Vérification numérique ; Validation expérimentale

1. Introduction

Hyperelastic damage modeling has been investigated in past years by several authors dealing with elastomeric materials. Most of the derived models are phenomenological in nature and generally consist in an adaptation of Continuum Damage Mechanics (CDM) concepts already derived for other class of materials. Mention can be made of works by Ogden and Roxburgh [1] based on a pseudo-elasticity approach. In the field of homogenization theory, an evolving damage model has been proposed by Govindjee and Simo [2] based on the very simple Voigt approximation (see also [3] dealing with Mullins damage). Brieu and Devries [4] investigated the damage phenomenon in the case of periodic microstructures.

The present work is devoted to a modeling of damage in hyperelastic materials with random microstructure. The principal objective is to derive a new isotropic damage model based on recent developments in the field of nonlinear homogenization. To this end, we adopt the second order method, introduced by P. Ponte Castañeda [5] and applied later to hyperelastic composites by [6] for random microstructures and by [7] for periodic ones. Applications of this method to porous hyperelastic materials have been recently done by [8]. We first present and implement in the 3D context the method in the case of porous hyperelastic materials, the voids being spherical. Then, we verify its predictions by comparing them to Finite Elements simulations on a unit cell. Taking advantage of the fact that the obtained macroscopic strain energy density of the porous hyperelastic material depends on the macroscopic deformation gradient $\bar{\mathbf{F}}$ and on the material porosity c , we propose a full 3D isotropic damage model based on the porosity evolution.¹ This model is obtained by combining the second order homogenization method with standard thermodynamics arguments. The predictions of the micro-macro damage model are then shown for a first validation on an EPDM/PP composite previously studied in [9] by means of a micromechanical model which does not account for damage. An example of cyclic behavior is also presented.

2. The second order homogenization method: principle and implementation for 3D hyperelastic porous materials

Consider a representative elementary volume (R.E.V.), denoted Ω_0 , and composed of an hyperelastic matrix weakened by a random distribution of voids. This R.E.V. is assumed to occupy a volume V_0 in the reference configuration and to satisfy the standard scale separation conditions. The porous material is subjected to homogeneous boundary strain conditions: $\underline{u} = (\bar{\mathbf{F}} - \mathbf{I}) \cdot \underline{X}$ on $\partial\Omega_0$. The heterogeneous deformation gradient tensor \mathbf{F} satisfies then $\bar{\mathbf{F}} = \langle \mathbf{F} \rangle$ with $\langle \cdot \rangle$ the volume average over Ω_0 . The local behavior of the hyperelastic solid matrix is defined by a strain energy density $W^{(1)}(\mathbf{F})$ while the microcavities are described by $W^{(r)}(\mathbf{F}) = 0$ ² ($r = 2, \dots, N$). It has been shown by Hill [10] that the homogenized constitutive law, giving the macroscopic first Piola–Kirchhoff stress tensor $\bar{\mathbf{T}} = \langle \mathbf{T} \rangle$, is determined by a macroscopic strain energy density \tilde{W} such that:

$$\bar{\mathbf{T}}(\bar{\mathbf{F}}) = \frac{\partial \tilde{W}(\bar{\mathbf{F}})}{\partial \bar{\mathbf{F}}} \quad (1)$$

In order to assess the homogenized energy in the case of nonlinear materials, various approaches are developed in Ponte Castañeda and Suquet [11]. In particular, the second order homogenization procedure which provides estimates of \tilde{W} , is based on a linearization of the strain energy densities of each phase, $W^{(r)}(\mathbf{F})$, by using a Taylor expansion.

Let us consider now an hyperelastic matrix containing a unique population of voids, denoted by ‘2’. For this two-phase hyperelastic composite, denoting by $\mathbf{T}^{(1)}(\bar{\mathbf{F}}^{(1)}) = \frac{\partial W^{(1)}}{\partial \mathbf{F}}(\bar{\mathbf{F}}^{(1)})$ and c the porosity, the second order method (see [6]) can be specialized and provides the following estimate of the macroscopic strain energy density:

$$\tilde{W}(\bar{\mathbf{F}}) \simeq (1 - c) \left\{ W^{(1)}(\bar{\mathbf{F}}^{(1)}) + \frac{1}{2} (\bar{\mathbf{F}} - \bar{\mathbf{F}}^{(1)}) : \mathbf{T}^{(1)}(\bar{\mathbf{F}}^{(1)}) \right\} \quad (2)$$

¹ Effects of voids shape change are disregarded.

² The superscript (r) stands for a family r of microcavities.

The macroscopic stress tensor, given by the derivative of (2) with respect to $\bar{\mathbf{F}}$, is then estimated by:

$$\bar{\mathbf{T}}(\bar{\mathbf{F}}) = \frac{1-c}{2} \left[\mathbf{T}^{(1)}(\bar{\mathbf{F}}^{(1)}) + [\mathbf{T}^{(1)}(\bar{\mathbf{F}}^{(1)}) + \mathbb{L}^1(\bar{\mathbf{F}}^{(1)}) : (\bar{\mathbf{F}} - \bar{\mathbf{F}}^{(1)})] : \frac{\partial \bar{\mathbf{F}}^{(1)}}{\partial \bar{\mathbf{F}}} \right] \tag{3}$$

where $\mathbb{L}^1(\bar{\mathbf{F}}^{(1)}) = \mathbb{L}_r^1(\bar{\mathbf{F}}^{(1)}) = \frac{\partial^2 \mathbf{W}^{(1)}}{\partial \mathbf{F} \partial \mathbf{F}}(\bar{\mathbf{F}}^{(1)})$.

Note that the only unknown in (3) is the average deformation gradient in phase 1, $\bar{\mathbf{F}}^{(1)}$, which may be computed from the resolution of a thermoelastic problem linked to a linear comparison composite involved in the method. In the case of two-phase materials, the resolution of this thermoelastic problem is performed thanks to the Levin’s theorem [12] which reads in the case of porous media:

$$\bar{\mathbf{F}}^{(r)} = \mathbb{A}^{(r)}(\bar{\mathbf{F}}^{(r)}) : \bar{\mathbf{F}} + (\mathbb{A}^{(r)}(\bar{\mathbf{F}}^{(r)}) - \mathbb{I}) : (\mathbb{L}^{(1)}(\bar{\mathbf{F}}^{(1)}))^{-1} : \boldsymbol{\tau}^{(1)}(\bar{\mathbf{F}}^{(1)}); \quad r = 1, 2 \tag{4}$$

where $\boldsymbol{\tau}^{(1)} = \mathbf{T}^{(1)}(\bar{\mathbf{F}}^{(1)}) - \mathbb{L}^1 : \bar{\mathbf{F}}^{(1)}$ is a polarization tensor which can be seen as a fictitious thermal stress and $\mathbb{A}^{(r)}$ is the localization tensor associated to phase (r) in the linear comparison composite.

In the present study, taking into account the matrix-inclusion type morphology of the (porous) material, we will consider the well-known Hashin–Shtrikman bound [13]. The micromechanical model will be then referred as HS-based model.

Note. For the Hashin–Shtrikman bound, due to the dependence of the localization tensors (and therefore of $\bar{\mathbf{F}}^{(1)}$) on c , expression (2) of the macroscopic strain energy density may depend nonlinearly on c . Comparatively, the Voigt model, which corresponds to an assumption of uniform strain in the material ($\bar{\mathbf{F}}^{(1)} = \bar{\mathbf{F}}^{(2)} = \bar{\mathbf{F}}$), provides the following estimate, $\tilde{\mathbf{W}}(\bar{\mathbf{F}}) \simeq (1 - c)\mathbf{W}^{(1)}(\bar{\mathbf{F}})$, linear with c .

For the implementation of the nonlinear micromechanical model of porous materials, some specific points need to be clarified. First, due to the anisotropy of $\mathbb{L}^{(1)}$, it is necessary to compute numerically the Hill tensor \mathbb{P} (required in the determination of the Hashin–Shtrikman bound). This is done by means of a Gaussian integration technique used for the numerical integration over the surface of the unit sphere $|\xi| = 1$. Secondly, as already indicated, a fictitious thermoelasticity problem have to be solved in order to determine the average deformations $\bar{\mathbf{F}}^{(1)}$ and $\bar{\mathbf{F}}^{(2)}$ of the two-phase linear comparison composite material. From a practical point of view, it is only necessary to determine $\bar{\mathbf{F}}^{(1)}$ to compute the macroscopic stress tensor (3), $\bar{\mathbf{F}}^{(2)}$ being deduced from the standard average rule: $\bar{\mathbf{F}} = c^{(1)}\bar{\mathbf{F}}^{(1)} + c^{(2)}\bar{\mathbf{F}}^{(2)}$. The resolution of the nonlinear system (4) is performed by using a Newton–Raphson method (cf. [14]). Moreover, due to the absence of a closed-form expression for \mathbb{P} , the Jacobian matrix, \mathbf{J} , needed in the Newton–Raphson method, cannot be analytically determined. Consequently, a numerical derivation by finite difference with the iterative scheme of Ridders–Richardson was used. This scheme is based on an algorithm in which a control and optimization of the numerical errors are performed at each step of the derivation procedure (see [14]). Once the resolution of the problem achieved, it is possible to compute the macroscopic stress from (3). To this end, the derivative of $\bar{\mathbf{F}}^{(1)}$ with respect to $\bar{\mathbf{F}}$ has yet to be determined.

3. Numerical verification by Finite Elements simulations

In order to provide a verification of the model based on the second order method, we present in this section some comparisons with reference solutions obtained by Finite Elements (FE) calculations. To this end, the same assumptions on the local constituents in both homogenization and FE simulations will be considered. The FE reference solution is obtained by considering a cylindrical unit cell representing the porous medium. As illustrated on Fig. 1, the space is supposed filled by prisms with hexagonal basis which represent the matrix, each prism containing an inclusion in its center. This procedure is similar to that already followed by various authors for composites materials (see for instance [15]) and allows us to consider different types of inclusions: rigid or deformable ones but also cavities, by considering for each case the suitable parameters in the strain energy density used to describe their behavior.

To take advantage of symmetry, the 3D unit cells are approximated by cylinders with circular basis to allow axisymmetric computations. Thus, the displacement boundary conditions considered for the simulation of a uniaxial tensile test are the following:

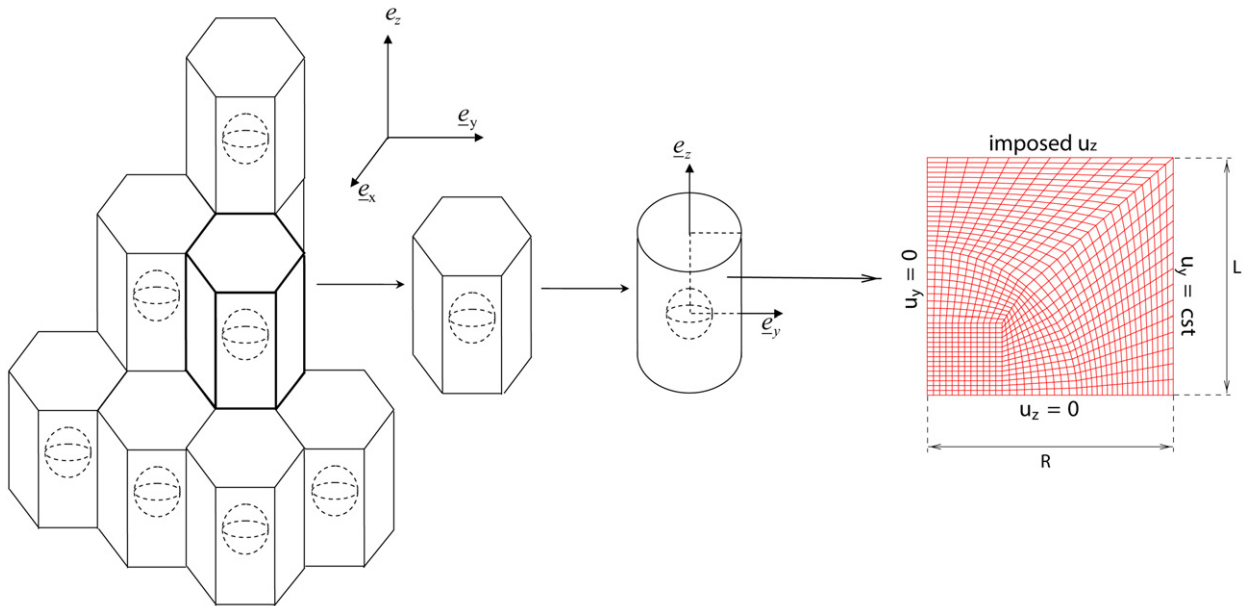


Fig. 1. A periodic network of hexagons with pores; reduction to a 2D axisymmetric unit cell.

- $U_z(y, 0) = 0, 0 < y < R$
- $U_z(y, L) = U_z \text{ imposed}, 0 < y < R$
- $U_y(0, z) = 0, 0 < z < L$
- $U_y(R, z) = \text{constant}, 0 < z < L$

The last condition yields the same radial displacement for points at the lateral boundary; the value of this displacement is obtained as the result of the Finite Element computation.

The FE simulations have been performed using the software Abaqus; the unit cell used contains CAX8R elements (8-node biquadratic axisymmetric quadrilaterals, with reduced integration). These FE simulations provide heterogeneous strain and stress fields in the unit cell from which can be computed their volume average by using a specific post-treatment script. Since our strategy is to compare the model predictions, first to numerical (FE) computations on the unit cell and then to experimental data on an EPDM/PP composite (an elastomer (EPDM) reinforced by Polypropylene particles (PP)), we have chosen for the matrix phase a suitable strain energy density $W^{(1)}$, proposed by Diani-Lambert and Rey [16]³ and for the voids, a Neo-Hookean hyperelastic model $W^{(2)}$ available in the software Abaqus. These densities are expressed as functions of the standard invariants (I_1, I_2, I_3) of the dilatation tensor $\mathbf{C} = \mathbf{F}^t \mathbf{F}$:

$$W^{(1)}(\mathbf{F}) = \int_3^{I_1} e^{(\alpha_0 + \alpha_1(I_1 - 3) + \alpha_2(I_1 - 3)^2)} dI_1 + \int_3^{I_2} \beta_1 I_2^{\beta_2} dI_2 \quad (5)$$

where $\alpha_0, \alpha_1, \alpha_2, \beta_1, \beta_2$ are the model parameters for the matrix phase which have to be identified for the considered EPDM.

$$W^{(2)}(\mathbf{F}) = C_{10}(J^{-2/3} I_1 - 3) + \frac{1}{D_1}(J - 1)^2 \quad (6)$$

where $J = \sqrt{I_3}$ and the model parameters are taken so as to model a void by an infinitely soft material: $C_{10} \rightarrow 0$ and $D_1 \rightarrow \infty$. In practice, we have considered $C_{10} = 10^{-5}$ MPa and $D_1 = 10^4$ MPa⁻¹.

³ According to [16], the density (5) is adequate for the modeling of the behavior of elastomers even for high elongation.

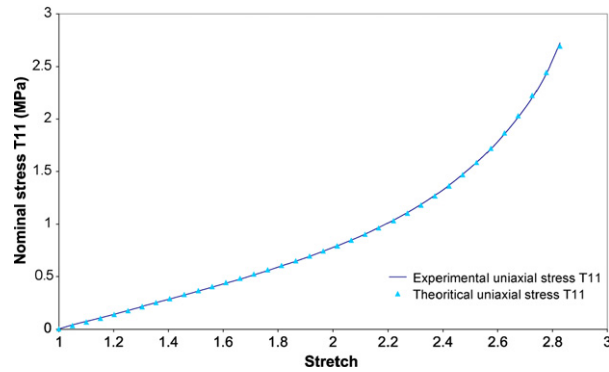


Fig. 2. Result of the identification of the Lambert-Diani and Rey density for the EPDM matrix.

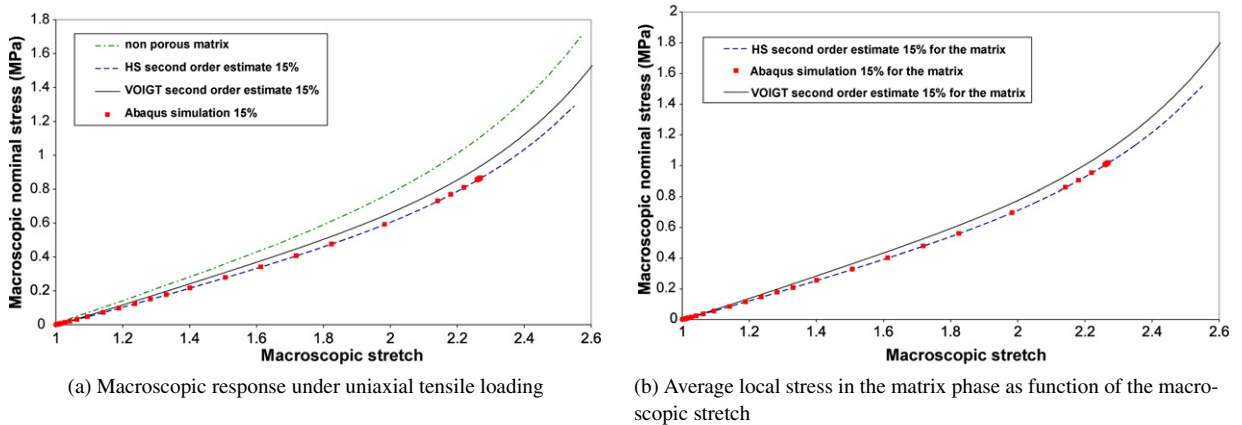


Fig. 3. HS-based model predictions compared to the numerical response for the hyperelastic material with 15% of porosity.

The result of the identification procedure for the considered EPDM, shown on Fig. 2, provides the following values of the parameters: $e^{\alpha_0} = 0.2246$ MPa; $\alpha_1 = 0.013051$; $\alpha_2 = 0.024$; $e^{\beta_1} = 0.38104$ MPa; $\beta_2 = -2.03234$.

Since the energy density of type (5) is not available in the Abaqus, we have first proceeded to its implementation in this software via the user routine UMAT. For the purpose of comparison, a porosity of 15% is considered. The comparison between the predicted macroscopic behavior and the results computed from the FE solution, shown on Fig. 3(a), indicates a good agreement which is confirmed by the comparison of the local average stresses in the matrix phase (see Fig. 3(b)). It is also interesting to investigate the strain field induced in the porous material by the tensile loading (see Fig. 4(a)). Although a significant heterogeneity of the strain is observed, it appears that the homogenization method provides a very accurate estimate of the average deformation in the solid matrix phase (see comparison on Fig. 4(b)).

4. A damage model based on the second order homogenization method

We aim now at deriving a damage model based on the nonlinear homogenization method applied in the above sections to hyperelastic porous materials. The starting point is that in contrast to the previous sections, the porosity may be considered now as a quantity which evolves irreversibly. We consider then the micromechanical estimate (2) of the macroscopic density as the thermodynamical potential of the damage material. It is readily seen that the porosity c can be considered as the internal damage variable which enters together with $\bar{\mathbf{F}}$ in the definition of the potential: $\tilde{W}(\bar{\mathbf{F}}, c)$. Obviously, it comes that in contrast to purely macroscopic approaches, the homogenization method provides not only a clear physical interpretation of the damage variable, but also gives us the expression of \tilde{W} , i.e. the way the damage affects the material behavior. As already stated, this expression strongly depends on the homogenization scheme used for the resolution of (4).

$F_{macro11}=2.3$

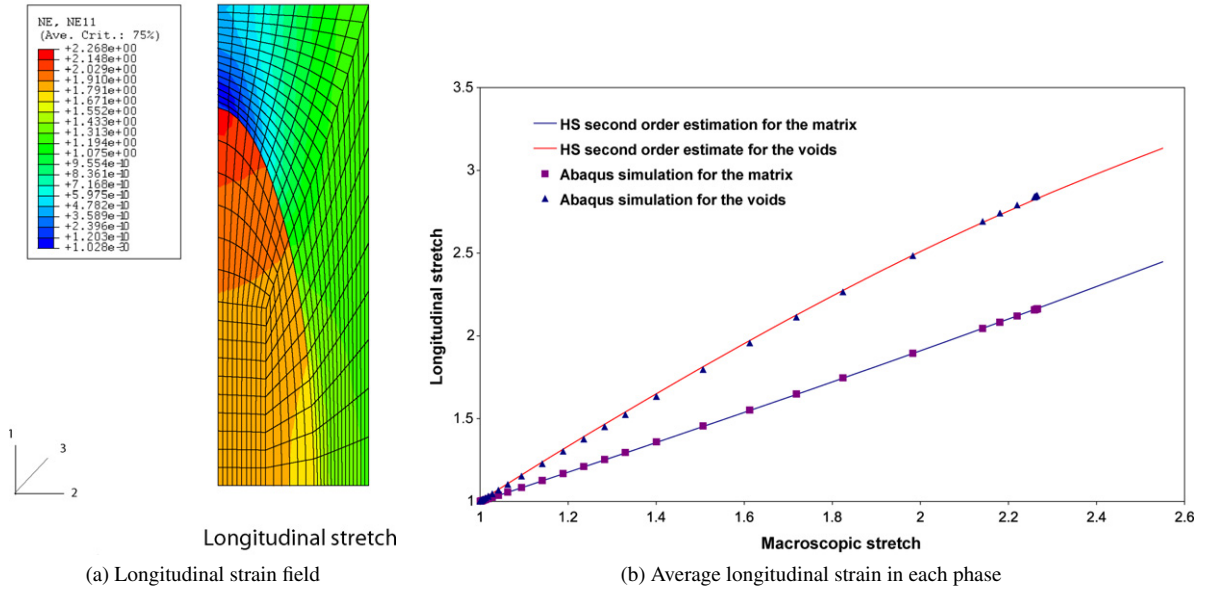


Fig. 4. Predictions of the HS-based model compared to the numerical response (15% of porosity).

4.1. Description of the damage model

As classically, the first state law, derived from \tilde{W} , reads similarly to (3) as: $\bar{T}(\bar{F}, c) = \frac{\partial \tilde{W}(\bar{F}, c)}{\partial \bar{F}}$. The thermodynamical force, \mathcal{F} , associated to the damage variable c , is given by the second state law:

$$\mathcal{F} = - \frac{\partial \tilde{W}(\bar{F}, c)}{\partial c}$$

$$\mathcal{F} = W^{(1)}(\bar{F}^{(1)}) + \frac{1}{2}(\bar{F} - \bar{F}^{(1)}) : \mathbf{T}^{(1)}(\bar{F}^{(1)}) - \frac{1-c}{2}[\mathbf{T}^{(1)}(\bar{F}^{(1)}) + (\bar{F} - \bar{F}^{(1)}) : \mathbb{L}^1(\bar{F}^{(1)})] : \frac{\partial \bar{F}^{(1)}}{\partial c} \tag{7}$$

Although, the Hashin–Shtrikman bound is the principal homogenization scheme used in the study, it is interesting to point out that for the Voigt scheme, the macroscopic stress, $\bar{T}(\bar{F}, c) = (1 - c)\mathbf{T}^{(1)}(\bar{F})$, depends linearly on c and the thermodynamical force, $\mathcal{F} = W^{(1)}(\bar{F})$, is not affected by the damage variable (porosity). Note that this very simple damage model, associated with the Voigt scheme, was the one proposed by Govindjee and Simo [2] and extended in many variants by several authors [1] (for a pseudo-elasticity approach), [3] etc.

The next step is to specify the damage evolution law, i.e. the cavity growth process. For the coherence of the approach, this evolution law should be also deduced from micromechanical considerations. Since, until now, there is no theoretical or physical arguments to do this, the methodology followed here consists to combine the micromechanical approach with standard thermodynamic arguments related to the analysis of the intrinsic dissipation when damage phenomena occur. Indeed, noting that the positivity of the intrinsic dissipation reduces to $\mathcal{F} \frac{\partial c}{\partial t} \geq 0$, one postulates the existence of a dissipation pseudo-potential $\phi^*(\mathcal{F})$ differentiable, convex, positive, zero for $\mathcal{F} = 0$ and such that:

$$\frac{\partial c}{\partial t} = \frac{\partial \phi^*}{\partial \mathcal{F}} \tag{8}$$

Following Brieu [17] a Norton type form of the dissipation pseudo-potential is adopted:

$$\phi^*(\mathcal{F}) = \frac{\alpha}{\beta + 1} \mathcal{F}^\beta, \quad \alpha \geq 0, \beta \geq 0 \tag{9}$$

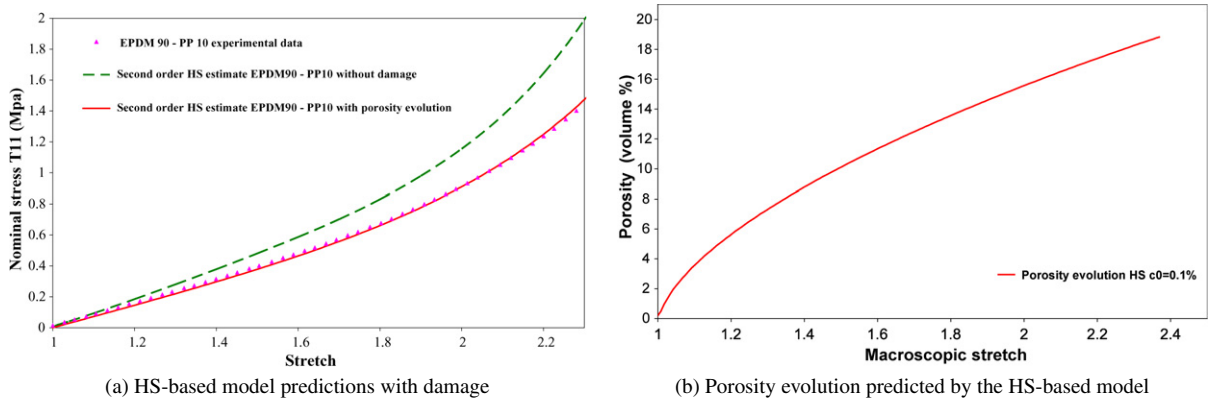


Fig. 5. Uniaxial tensile test for the EPDM 90–PP 10 with an initial porosity of 0.1%.

4.2. Implementation and results

Implementation of the proposed damage model requires a simultaneous resolution of the homogenization problem and of the damage evolution. For this, we adopt a method separating the space problem i.e. the homogenization one and the temporal problem of damage evolution. Thus, the solution is obtained at a time t by continuity of two successive steps: for an initial porosity $c_0(t)$ and an imposed deformation gradient tensor $\bar{\mathbf{F}}(t)$, we compute $\tilde{\mathbf{W}}(\bar{\mathbf{F}}(t), c_0(t))$ and $\bar{\mathbf{T}}(\bar{\mathbf{F}}(t), c_0(t))$ by resolving the homogenization problem. After this, we can evaluate the porosity $c_1(t)$ thanks to the evolution law (8) and compute once again $\tilde{\mathbf{W}}(\bar{\mathbf{F}}(t), c_1(t))$ and $\bar{\mathbf{T}}(\bar{\mathbf{F}}(t), c_1(t))$. A convergence test is performed for the porosity (i.e. $|c_1(t) - c_0(t)| \leq \varepsilon$ with ε very small); if the convergence is not obtained, we continue the successive steps in order to converge for an iteration k : $|c_k(t) - c_{k-1}(t)| \leq \varepsilon$. In this algorithm, the homogenization problem is solved as described previously in Section 2 and the porosity $c(t)$ is determined thanks to the integration of the evolution law (8) based on (9):

$$c(t) = c(0) + \frac{\alpha}{\beta + 1} \int_0^t \mathcal{F}(t)^{(\beta-1)} dt \tag{10}$$

To compute $c(t)$, we choose to use a trapezoidal rule. Thus, the damage evolution during a interval of time $[0, T]$ is determined by considering intermediate times t_j for which we compute the macroscopic stresses and the damage (porosity) of the material. These intermediate times are defined by $t_j = j\Delta t = j\frac{T}{N}$ ($j = 1, \dots, N$), N being the number of sub-intervals in $[0, T]$ which have to be small enough to for the desire accuracy. The evaluation of the porosity at each time t_j is then determined from the following approximation given by the trapezoidal rule:

$$c(t_j) = c_0 + \frac{\alpha}{\beta + 1} \left(\mathcal{F}(t_j)^{(\beta-1)} + 2 \sum_{i=1}^{j-1} \mathcal{F}(i\Delta t)^{(\beta-1)} \right) \tag{11}$$

Let us consider now the composite EPDM/PP for which experimental data are available (see our previous study [9]). It was also shown in [9] that a micromechanical model of composite, without damage, is not able to reproduce the macroscopic experimental behavior. Our objective here is simply to apply the damage model derived here to the EPDM/PP. The methodology followed consists in a two step homogenization: i) we first homogenize the EPDM/PP in order to obtained its macroscopic behavior in absence of damage; ii) we then consider this macroscopic behavior as the one of the solid matrix in the second homogenization step devoted to the damage modeling. In this second step of homogenization the initial porosity is considered very low (0.1%).

For the pseudo-potential ϕ^* , parameters α and β are calibrated on the data from the material made up of 90% of EPDM and 10% of PP particles: $\alpha = 1 \times 10^{-4}$ and $\beta = 0.8$. Fig. 5(a), which shows the results given by the damage model based on the Hashin–Shtrikman (HS) bound with the experimental data, confirms the relevance of the identification. For completeness, the predictions of the model without damage phenomenon are also presented. A clear effect of the damage is observed and makes it possible to describe the experimental behavior.

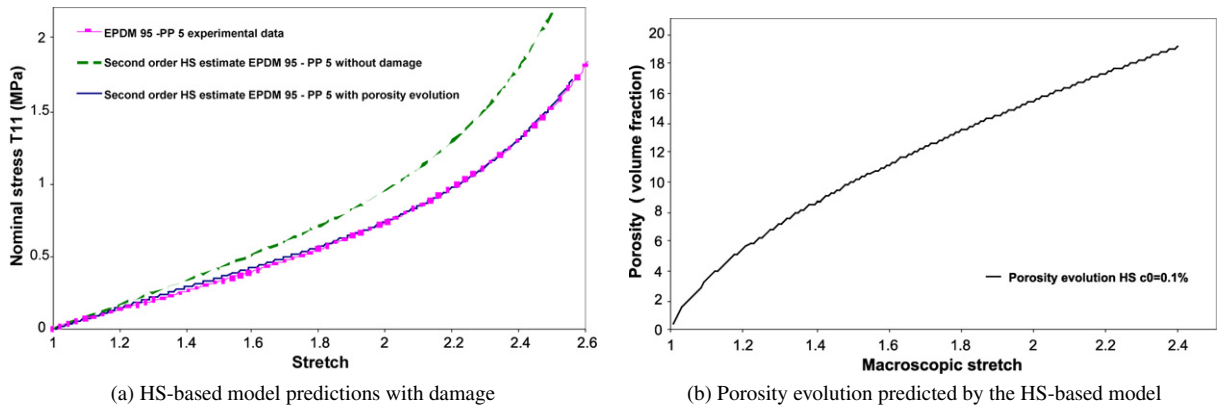


Fig. 6. Uniaxial tensile test for the EPDM 95–PP 5 with an initial porosity of 0.1%.

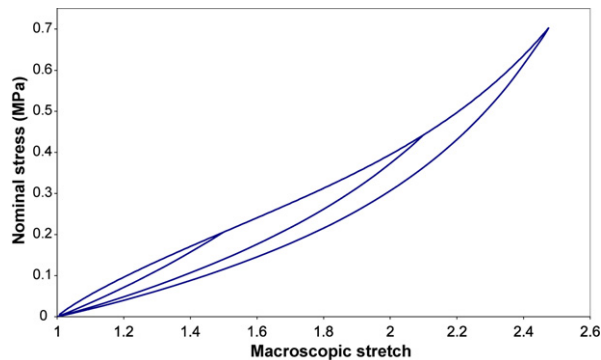


Fig. 7. Cyclic behavior of the EPDM 90–PP 10 composite with evolving damage.

For validation purposes, another blend EPDM/PP made up now of 95% of EPDM and 5% of PP particles is considered. The comparison of the predictions to experimental data (see Fig. 6(a)) shows an agreement which demonstrates the predictive capabilities of the proposed model. The damage evolution during the loading is also presented on Figs. 5(b) and 6(b) for the two considered blends EPDM/PP. It is observed that for the maximum level of deformation in the test, the damage value is quite equal to 18%. For further details, one can refer to Bouchart [18]

Finally, the cyclic behavior of the composite in the presence of an evolving damage is presented on Fig. 7. For the clarity of the illustration, we have considered for this simulation: $\alpha = 4 \times 10^{-4}$ and $\beta = 0.65$. The obtained behavior appears as the consequence of the irreversibility of the damage process. Note that these cycles are obtained without any viscosity effects and no attempt is made here to reproduce hysteresis phenomena observed in elastomeric materials.

5. Conclusion

The modeling of damage phenomena in hyperelastic materials has been investigated in the present note by means of the second order homogenization method. We first provide a verification of this method combined with a Hashin–Shtrikman bound by comparing its predictions to results obtained from Finite Elements calculations on a unit cell. The formulation of the damage model is obtained by combining the micromechanical results with a standard thermodynamics-based reasoning. A first validation is provided through the comparison of the model predictions with experimental data obtained on an EPDM/PP. Investigations on the cyclic behavior of the damaged material also allowed to illustrate the macroscopic effects of the damage phenomenon.

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