

Macroscopic analysis of heterogeneous solids including the effects of finite changes in constitutive and geometric microstructural properties

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Keywords: Homogenization, Stability, Heterogeneous microstructure

SUMMARY. A relevant aspect in the study of solids with heterogeneous microstructure is the analysis of microscopic instability phenomena by using their macroscopic properties. To this end a stability analysis on the micro and macro scales is here carried out in order to investigate macroscopic stability conditions able to predict microscopic instability mechanisms in composite solids with periodic microstructure. The macroscopic stability conditions are formulated in terms of positive definiteness of the homogenized moduli tensors associated to specific conjugate stress-strain pairs. Numerical applications, devoted to cellular and fiber-reinforced composite microstructures with hyperelastic constituents, are developed by implementing a one way coupled finite element approach. The ability of the proposed macroscopic measures is examined by means of comparisons between the exact microscopic stability region in the macro-strain space, obtained by taking into account microstructural details, and the macroscopic stability regions, determined by investigating the homogenized material properties.

1 INTRODUCTION

A notable aspect in the study of solids with heterogeneous microstructure is the analysis of microscopic instability phenomena by using their macroscopic properties. As a matter of fact, microscopic failure mechanisms in composite materials are often induced by instability phenomena and the stability analysis allows to define the region of validity of the standard homogenization procedure based on the one cell analysis [1-3]. A direct stability analysis taking into account a precise description of microstructural details may involve a notable computational effort since nonlinear effects related to the microgeometry and the local constitutive law must be incorporated in the mathematical model.

For solids with generic microstructures, such as composite materials, the analysis must consider both classical buckling type instability modes dominated by the geometric microstructural configuration when the stress state is prevalently negative, and constitutive-dominated instabilities occurring when tangent moduli of the material reduce greatly taking eventually negative values and in presence of a positive stress state. Instabilities of the former kind arise frequently in laminated microstructures loaded primarily in compression due to fiber micro-buckling [4], whereas cellular and fiber-reinforced microstructures may exhibit the latter kind of instability when loaded prevalently in tension [3,5].

In the sake of computational efficiency, the stability analysis of elastic composite solids with periodic microstructure is carried out in terms of their macroscopic properties. However, a stability analysis based on the homogenized constitutive properties may be not able to provide an accurate prediction of microscopic instability mechanisms. Consequently, the analysis of the interrelations between instabilities on the macro and micro scales plays a fundamental role to justify a stability investigation based on the homogenized composite properties. Several measure of stability based on homogenized constitutive properties can be adopted. A fundamental one is based on the strong

ellipticity condition of the homogenized moduli tensor [2]. This condition allows to obtain an upper bound beyond which the microstructure is surely unstable, thus providing a unconservative prediction of the primary microscopic instability load.

In order to investigate alternative macroscopic conditions able to obtain accurate prediction of the microscopic instability mechanisms in composite solids with periodic microstructure, a stability analysis on the micro and macro scales is here carried out, both from a theoretical and numerical point of views. Numerical applications, devoted to cellular and fiber-reinforced composite microstructures with hyperelastic constituents, are developed by implementing a oneway coupled finite element approach, in which the finite strain boundary value problem needed to determine the evolution of the deformed microstructure configuration, the incremental boundary value problem necessary to evaluate homogenized tangent moduli and the linearized eigenvalue problem giving the microscopic primary instability load, are solved sequentially.

Comparisons between the exact microscopic stability region in the macro-strain space, obtained by taking into account microstructural details, and the macroscopic stability regions, determined by investigating the homogenized material properties, are developed to examine the effectiveness of the proposed macroscopic stability measures.

2 THE MODEL

In order to analyze the stability problem of heterogeneous solids with periodic microstructure subjected to finite-strains loading conditions, microscopic and macroscopic stability conditions are here introduced. The former requires the examination of perturbations of the equilibrium fluctuation field, periodic over an a-priori unknown unit cell assembly, whereas the latter involves calculations over a unit cell. Additional details on the derivation of micro- and macroscopic stability conditions can be found in [6].

2.1 Microstructural stability

Let us consider an heterogeneous solid with a periodic microstructure defined by a unit cell occupying the domain V_i in the stress-free undeformed configuration. The material model is assumed to be rate independent and is specified by the following incrementally linear constitutive law:

$$\dot{\mathbf{T}}_R = \mathbf{C}^R(\mathbf{F}, \mathbf{X})[\dot{\mathbf{F}}] \quad (2)$$

where $\dot{\mathbf{T}}_R$ is the rate of the first Piola-Kirchhoff stress tensor, $\dot{\mathbf{F}}$ is the deformation gradient rate and \mathbf{C}^R is the corresponding fourth-order tensor of nominal moduli, a $V_{(i)}$ -periodic function of \mathbf{X} . It is further assumed that the nominal moduli tensor possesses major symmetry condition, i.e. $\mathbf{C}^R_{ijkl} = \mathbf{C}^R_{klij}$. The microscopic deformation $\mathbf{x}(\mathbf{X})$ at the material point \mathbf{X} , can be assumed to be a function of the macro-deformation gradient $\bar{\mathbf{F}}$ and can be expressed as the sum of a linear part and of a fluctuation field $\mathbf{w}(\mathbf{x})$ periodic on the unit cell boundary:

$$\mathbf{x}(\mathbf{X}) = \bar{\mathbf{F}}\mathbf{X} + \mathbf{w}(\mathbf{X}) \quad \bar{\mathbf{F}} = \frac{1}{|V_{(i)}|} \int_{\partial V_{(i)}} \mathbf{x}(\mathbf{X}) \otimes \mathbf{n}_{(i)} ds_{(i)} \quad (1)$$

Suppose that the microstructure at a generic stage of a quasi-static loading path $\bar{\mathbf{F}}(\beta)$ (with the load parameter $\beta \geq 0$ increasing monotonically with increasing macroscopic load) beginning from the initial configuration (i.e. with $\bar{\mathbf{F}}(\beta) = \mathbf{I}$ when $\beta = 0$) occupies a known region $k^N V$, where $k^N V$ denotes an ensemble of $k^N = [0, k]^N$ unit cells ($N=2$ or $N=3$ for 2D or 3D problems, respectively) with k an arbitrary integer. According to the infinitesimal static stability criterion, the deformed state $k^N V$ of the microstructure, characterized by the fluctuation field $\mathbf{w}(\mathbf{x})$ induced by the macroscopic load $\bar{\mathbf{F}}(\beta)$, is stable if the minimum eigenvalue of the stability functional is positive when the minimum is taken over all admissible incremental fluctuations periodic on the $k^N V$ ensemble of unit cells:

$$\Lambda(\bar{\mathbf{F}}) = \inf_{k \in \mathbb{N}} \left\{ \min_{\mathbf{w} \in H^{1,p}(k^N V_{\#})} \left\{ \frac{\int_{k^N V} \mathbf{C}_0^R(\mathbf{x}, \bar{\mathbf{F}} + \nabla \mathbf{w}_{\bar{\mathbf{F}}}) [\nabla \mathbf{w}] \cdot \nabla \mathbf{w} dV}{\int_{k^N V} \nabla \mathbf{w} \cdot \nabla \mathbf{w} dV} \right\} \right\} > 0, \quad (4)$$

where \mathbf{C}_0^R is the fourth-order tensor of nominal instantaneous moduli. The primary microscopic instability occurs at some load level β_c (termed microscopic critical load parameter) for which:

$$\Lambda(\beta_c) = 0, \quad \Lambda(\beta) > 0 \quad \text{for } 0 \leq \beta < \beta_c. \quad (5)$$

Therefore the primary instability is detected when the minimum eigenvalue first vanishes. For hyperelastic materials, the microscopic stability region $\beta \mid \Lambda(\bar{\mathbf{F}}(\beta)) > 0$, inside which the fundamental periodic solution, for which all cells deform identically, is unique, establishes also the region where the one-cell standard homogenized energy coincides with the correct one determined with respect to admissible fluctuation fields periodic over $k^N V$, namely $\Lambda(\bar{\mathbf{F}}(\beta)) > 0$ implies $\bar{W}(\bar{\mathbf{F}}) = \bar{W}^1(\bar{\mathbf{F}})$ (see [2] for additional details), where:

$$\bar{W}(\bar{\mathbf{F}}) = \inf_{k \in \mathbb{N}} \left\{ \min_{\mathbf{w} \in H^{1,p}(k^N V_{i\#})} \left\{ \frac{1}{k^N |V_{(i)}|} \int_{k^N V_{(i)}} W(\mathbf{X}, \bar{\mathbf{F}} + \nabla \mathbf{w}) dV_{(i)} \right\} \right\}, \quad \bar{W}^1(\bar{\mathbf{F}}) = \min_{\mathbf{w} \in H^{1,p}(V_{i\#})} \left\{ \frac{1}{|V_{(i)}|} \int_{V_{(i)}} W(\mathbf{X}, \bar{\mathbf{F}} + \nabla \mathbf{w}) dV_{(i)} \right\} \quad (6)$$

As a matter of fact, due to instability phenomena it is possible that lower values for the homogenized strain energy function can be obtained by minimization over domains containing several unit cells. In this circumstance, eqn (6)₁ determines the current fluctuation field and defines the size of the representative volume of the microstructure which captures the minimizing micro-buckling mode.

2.2 Macroscopic stability measures

A microscopic stability analysis along a macroscopic loading path $\bar{\mathbf{F}}(\beta)$ requires a notable computational effort due to the infinity of the definition domain. As a consequence, it should be preferable to carry out the stability analysis of the heterogeneous solid in terms of its macroscopic properties determined by means of calculations performed on a unit cell. A basic macroscopic measure of the stability of the periodic solid at the load parameter β can be defined as the strong ellipticity condition of the homogenized moduli tensor:

$$\bar{\Lambda}(\bar{\mathbf{F}}(\boldsymbol{\beta})) = \min_{\|\bar{\mathbf{m}}\|=\|\bar{\mathbf{n}}\|=1} \left\{ \bar{\mathbf{C}}_0^R(\bar{\mathbf{F}}, \bar{\mathbf{X}})(\bar{\mathbf{m}} \otimes \bar{\mathbf{n}}) \cdot \bar{\mathbf{m}} \otimes \bar{\mathbf{n}} \right\} > 0, \quad (6)$$

in which the minimum is taken over all unit vectors $\bar{\mathbf{m}}$ and $\bar{\mathbf{n}}$. A macroscopic primary instability load associated to the stability condition (6) can be defined as $\bar{\Lambda}(\beta_{cM}) = 0$, $\bar{\Lambda}(\beta) > 0$ for $0 \leq \beta < \beta_{cM}$, where β_{cM} is the macroscopic critical parameter and, consequently, the macroscopic stability region $\beta \mid \bar{\Lambda}(\beta) > 0$ can be determined. In eqn (6) $\bar{\mathbf{C}}_0^R$ is the instantaneous homogenized moduli tensor, obtained by using the usual continuum relations from the fixed reference homogenized moduli tensor, whose components can be determined as

$$\bar{C}_{ijhk}^R(\bar{\mathbf{F}}) = \frac{1}{|V_{(i)}|} \int_{V_{(i)}} C_{ijmn}^R(\bar{\mathbf{F}}, \mathbf{X}) [I_{mn}^{hk} + \nabla \dot{w}_{hk}] dV_{(i)}. \quad (7)$$

Eqn (7) is expressed in terms of the incremental fluctuation field \dot{w}_{hk} induced by unit value for each component of the macroscopic deformation increment, namely the solution of the incremental boundary value problem for $\bar{\mathbf{F}} = \mathbf{I}^{hk}$ superimposed to the examined finitely strained equilibrium configuration defined by $\bar{\mathbf{F}}(\boldsymbol{\beta})$, where $I_{mn}^{hk} = \delta_{mh} \delta_{nk}$.

As proved in [2], the microscopic stability condition (4) implies the macroscopic stability condition (6), provided the microscopic material is strongly elliptic. Moreover, the primary microscopic instability can be detected as a loss of macroscopic stability (6) provided that the first instability is global in nature. On the contrary, for a local primary microscopic instability mode the macroscopic stability condition (6) still holds. It follows that an unconservative estimation of the primary microscopic instability load is obtained except for global instability modes.

As an alternative, the following family of macroscopic stability measures is introduced:

$$\bar{\Lambda}^f(\bar{\mathbf{F}}(\boldsymbol{\beta})) = \min_{\|\bar{\mathbf{D}}\|=1} \left\{ \bar{\mathbf{C}}_0^f(\bar{\mathbf{F}})[\bar{\mathbf{D}}] \cdot \bar{\mathbf{D}} \right\} > 0, \quad (8)$$

where $\bar{\mathbf{D}}$ is a symmetric tensor and $\bar{\mathbf{C}}_0^f$ is the macroscopic tensor of instantaneous homogenized moduli corresponding to the work conjugate stress-strain measure pair $(\mathbf{T}_f, \mathcal{A}(\mathbf{U}))$, based on strain measures coaxial with \mathbf{U} , the right stretch tensor associated to \mathbf{F} , and having principal values $f(\lambda_i)$ [7]. A specific macroscopic strain measure must be adopted in eqn (7) in order to define a unique stability measure. To this end a sub-class of stress-strain measure pairs corresponding to $f(\lambda_i) = (\lambda_i^m - 1)/m$, where m is an integer, is used. In the following numerical results the adopted values of m are -2, -1, 0, 1, 2 and the corresponding macroscopic stability measure are respectively denoted by: $\bar{\Lambda}^{(-2)}, \bar{\Lambda}^{(-1)}, \bar{\Lambda}^{(0)}, \bar{\Lambda}^{(1)}, \bar{\Lambda}^{(2)}$.

3 RESULTS

Applications to specific materials and specific microgeometries are here examined in order to numerically determine the critical load parameters associated to microscopic and macroscopic onsets of instability.

3.1 Numerical formulation and microstructural models

A one-way coupled FE model is formulated by using the commercial software COMSOL MULTIPHYSICS™, in order to compute sequentially respectively the principal solution path for

the unit cell, the incremental solutions needed to determine the homogenized tangent moduli and the minimum eigenvalue of the microscopic structural stability functional.

The finitely deformed configurations of a unit cell are determined along the principal equilibrium path for a given macroscopic loading process $\bar{\mathbf{F}}(\beta)$, assuming that the loading process produces a unique response. The solution is obtained by means of a parametric non-linear solver based on a continuation approach. The incremental equilibrium problems of the unit cell for each unit incremental macroscopic deformation mode are solved, superimposed on the given finite deformation along the loading path in order to compute the homogenized moduli by eqn (7). The load parameter associated to the lowest zero eigenvalue of the microscopic structural stability functional (4) must be computed over all possible ensemble of unit cells. From the computational point of view the linearized eigenvalue problem with a varying domain of definition is solved in the following simple way. For a fixed ensemble of unit cells the lowest value of β for which the minimum eigenvalue of the stability functional is zero is determined, namely β_c , together with the associated eigenmode by the discretization of the minimization problem (4). Then we successively enlarge the ensemble by increasing the number k . The minimum value of β_c for all currently possible instability modes then determines the optimal ensemble of unit cells. This value corresponds to the loss of microscopic stability. Finally the macroscopic stability analysis is performed by monitoring the lowest eigenvalue of the acoustic tensor $\bar{\mathbf{Q}}_{0ih}(\bar{\mathbf{n}}) = \bar{C}_{0ijk}^R \bar{n}_j \bar{n}_k$ for every direction of propagation $\bar{\mathbf{n}}$. The first macroscopic instability is detected when the lowest eigenvalue becomes zero. Similarly, the onset of macroscopic instability according to the conjugated stability measures is determined by monitoring the lowest eigenvalue of (8).

Periodic boundary conditions were implemented in the finite and incremental homogenization procedure by means of the extrusion coupling variable methodology. The evolution of the minimum eigenvalues of the microscopic and macroscopic stability conditions is managed by developing a computer code written in the COMSOLSCRIPT™ programming language, which is interfaced with COMSOL MULTIPHISICS™.

A compressible Gent constitutive law is adopted in numerical applications. The corresponding strain energy density is:

$$W = -\frac{\mu}{2} \left[J_m \ln \left(1 - \frac{\|\mathbf{F}\|^2 - 3}{J_m} \right) + 2 \ln J \right] + \left(\frac{k - \mu}{2} - \frac{\mu}{J_m} \right) (J - 1)^2, \quad (9)$$

where μ and κ are, respectively, the shear and bulk moduli of the solid at zero strain and J_m is a constant which calibrates the solid's strain saturation. The conditions $\mu > 0$, $\kappa > [(J_m + 2)/J_m] \mu$, $J_m > 0$ ensure that the strong ellipticity condition is satisfied for the microscopic material. The values of $J_m = 50$ and $\kappa/\mu = 10$ are adopted in the sequel.

A macroscopic uniaxial loading path is considered along the X_1 axis direction:

$$\bar{\mathbf{F}}(\beta) = \begin{bmatrix} 1 + \beta & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad (10)$$

In the first application, a cellular microstructure with an initial square distribution of circular voids is analyzed under plane strain conditions in the X_1 - X_2 plane. In the second one a particle

reinforced composite microstructure is considered with a square distribution of inclusions, which can be considered as representative of a cross section of a fiber-reinforced solid with cylindrical fibers aligned in the X_3 axis direction. In both cases the unit cell dimensions are $L_1=L_2=L$ and the radius of the voids and the inclusions is $R=0.25L$. In the numerical calculations the shear modulus at zero strain of the matrix material has been assumed equal to $\mu=807 \text{ N/mm}^2$.

The microscopic stability analysis involves an increasing assembly of unit cells. In the numerical calculations the largest assembly examined corresponds to an array of 20×20 unit cells. This assembly is assumed to be a reasonable approximation of the possibly infinite domain of microscopic stability analysis and provided values of the critical load parameter in the case of a global instability mode, sufficiently close to those obtained by using the macroscopic stability measure (6).

3.2 Cellular microstructure

The stability analysis is illustrated in Fig. 1 and shows that in compression the onset of microscopic instability (occurring at $\beta_c^- = -0.1435$) precedes the macroscopic loss of strong ellipticity and the local microscopic instability mode is periodic on a 2×2 cell assembly (see Fig. 2a), involving an alternation of void ovalization.

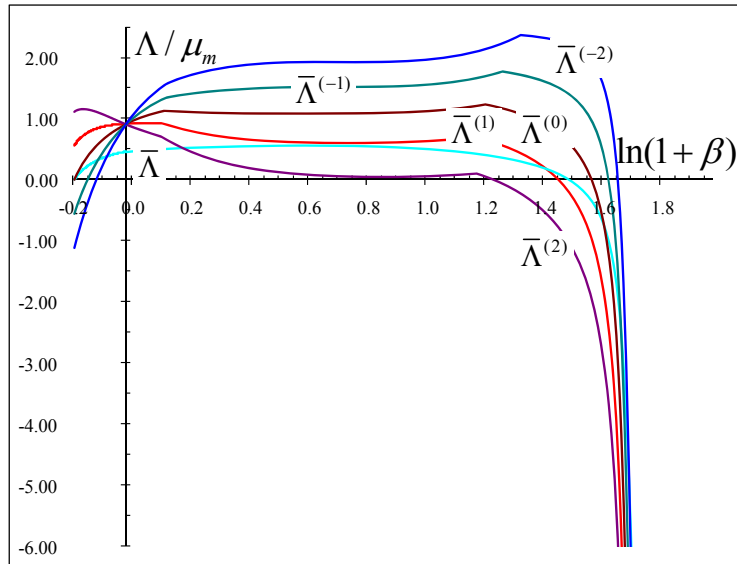


Figure 1: Stability analysis of a cellular microstructure.

In the tension case the first instability mode is global in nature as shown in Fig. 2b with reference to a 10×10 assembly and, consequently, the macroscopic loss of stability according to eqn (6) coincides with the microscopic one and occurs at $\beta_c^+ = 3.515$.

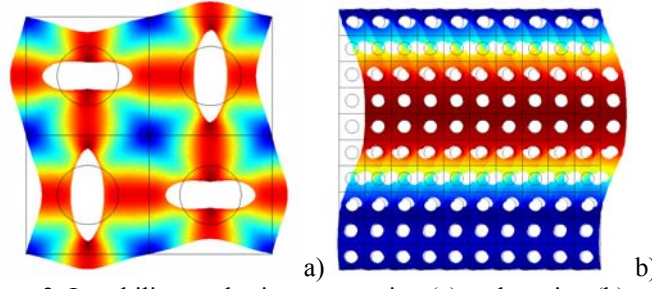


Figure 2: Instability modes in compression (a) and tension (b) case.

Numerical calculations have shown that in tension the conditions $\bar{\Lambda}^{(2)}$ and $\bar{\Lambda}^{(1)}$ are first violated before the macroscopic loss of strong ellipticity. On the contrary the loss of macroscopic conditions $\bar{\Lambda}^{(-1)}$ and $\bar{\Lambda}^{(-2)}$ occur after the macroscopic loss of strong ellipticity. In the compressive case, the situation is reversed since the loss of conditions $\bar{\Lambda}^{(-1)}$ and $\bar{\Lambda}^{(-2)}$ occur before the macroscopic loss of ellipticity, whereas the conditions $\bar{\Lambda}^{(2)}$ and $\bar{\Lambda}^{(1)}$ are first violated after the macroscopic loss of ellipticity. It is also possible to observe how the $\bar{\Lambda}^{(0)}$ condition is first violated after the macroscopic loss of ellipticity both in tension and in compression. In the examined range of macrostrain, the conditions $\bar{\Lambda}^{(2)}$ and $\bar{\Lambda}^{(1)}$ are not violated in compression, although show a decreasing behavior and tend to have a root for larger levels of strains. It follows that the $\bar{\Lambda}^{(2)}$ and $\bar{\Lambda}^{(1)}$ conditions provide conservative microscopic instability estimates in tension, whereas the conditions $\bar{\Lambda}^{(-1)}$ and $\bar{\Lambda}^{(-2)}$ provide conservative predictions in compression. The $\bar{\Lambda}^{(0)}$ condition always gives an unconservative microscopic instability load prediction. Among the proposed conjugated stability measures, the $\bar{\Lambda}^{(1)}$ and the $\bar{\Lambda}^{(-1)}$ conditions give the less conservative prediction of the microscopic critical load parameter in tension and compression, respectively.

3.3 Particle reinforced microstructure

In the case of the particle reinforced matrix ($\mu_f/\mu_m=0.5, 10, 50$), in the compression case the first microscopic instability mode is always of global type and coincides with the macroscopic instability related to the strong ellipticity condition. On the other hand, in tension the microstructure is always structurally stable for the examined range of deformations. The stability analysis, illustrated in Figs 3, 4 and 5, shows that in compression the onset of microscopic instability occurs at $\beta_c^-=-0.825$ for the $\mu_f/\mu_m=0.5$ case, at $\beta_c^-=-0.475$ for the $\mu_f/\mu_m=10$ case and at $\beta_c^-=-0.415$ for the $\mu_f/\mu_m=50$ case.

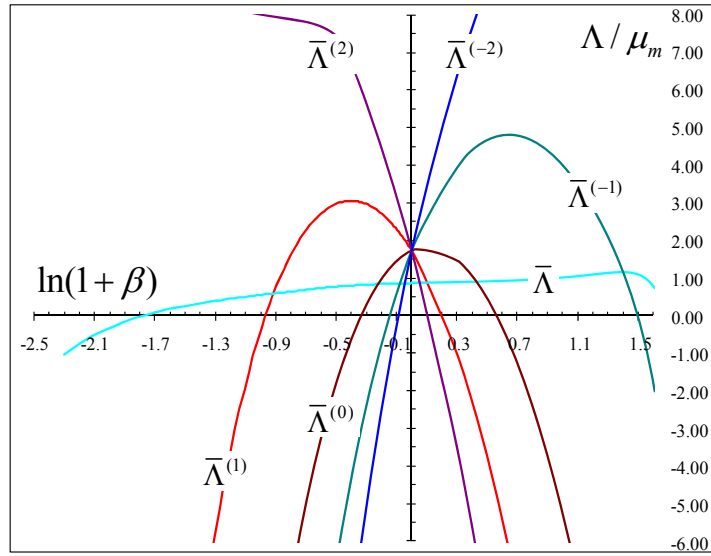


Figure 3: Stability analysis of a particle reinforced microstructure ($\mu_f/\mu_m=0.5$).

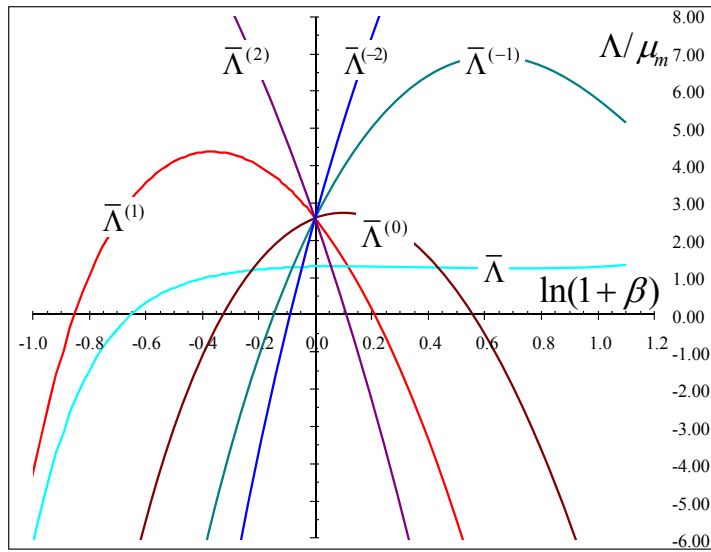


Figure 4: Stability analysis of a particle reinforced microstructure ($\mu_f/\mu_m=10$).

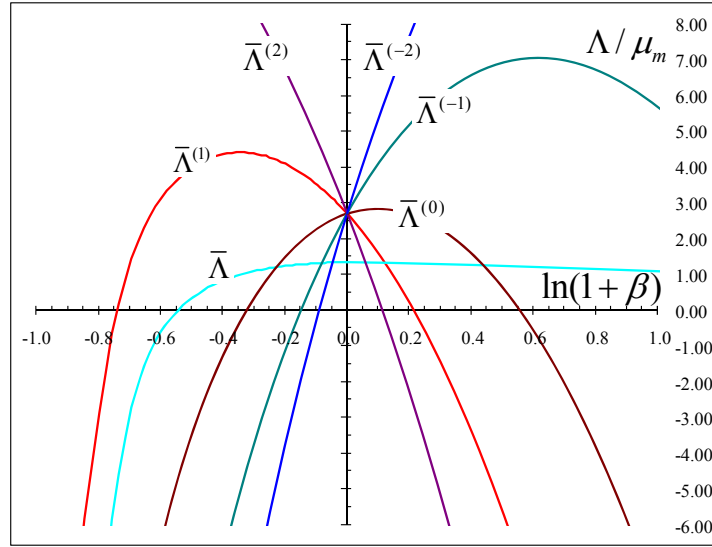


Figure 5: Stability analysis of a particle reinforced microstructure ($\mu_f/\mu_m=50$).

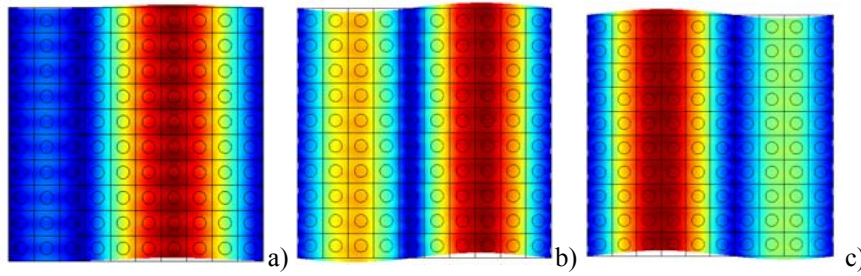


Figure 6: Instability modes in compression for (a) $\mu_f/\mu_m=0.5$, (b) $\mu_f/\mu_m=10$ and (c) $\mu_f/\mu_m=50$.

Fig. 6 shows one of the two simultaneous modes occurring in the analyzed macroscopic uniaxial compression case for $\mu_f/\mu_m=0.5$ (a), $\mu_f/\mu_m=10$ (b) and $\mu_f/\mu_m=50$ (c).

In compression, the loss of conditions $\bar{\Lambda}^{(-1)}$, $\bar{\Lambda}^{(-2)}$ and $\bar{\Lambda}^{(0)}$ occur always before the macroscopic loss of ellipticity. In addition in the case of the soft inclusion ($\mu_f/\mu_m=0.5$) the $\bar{\Lambda}^{(1)}$ condition is also violated before the $\bar{\Lambda}$ one. In the case of the stiff inclusion ($\mu_f/\mu_m=10, 50$) the $\bar{\Lambda}^{(-2)}$, $\bar{\Lambda}^{(-1)}$ and $\bar{\Lambda}^{(0)}$ conditions provide conservative microscopic instability estimates in compression. For the soft inclusion a conservative estimate in compression is also provided by the $\bar{\Lambda}^{(1)}$ condition.

Among the proposed conjugated stability measures and for the analyzed macrostrain range, the $\bar{\Lambda}^{(0)}$ give the less conservative prediction of the microscopic critical load parameter in tension and compression, for the stiff inclusion. On the other hand, for the soft inclusion the less conservative prediction is provided by the $\bar{\Lambda}^{(1)}$ and $\bar{\Lambda}^{(-1)}$ conditions in compression and tension, respectively.

The effect of inclusion, as expected, provides a stabilizing influence with respect to the cellular case.

4 CONCLUSIONS

The problem of estimating microscopic instability mechanisms in finitely strained composite materials with heterogeneous periodic microstructure by using macroscopic approaches based on the homogenization theory, is here studied. A class of macroscopic stability measures is introduced for incrementally linear materials based on the positive definiteness of homogenized moduli tensor associated with specific work conjugate stress-strain measures. A nonlinear procedure based on a one-way coupled finite element approach is developed in order to solve sequentially the unit cell principal equilibrium problem, the incremental equilibrium problems giving the homogenized tangent moduli and the stability eigenvalue problem along a prescribed monotonic macrostrain path. Numerical applications are then proposed with reference to a composite with circular inclusions and a cellular material adopting a compressible Gent strain energy function.

It is found that a conservative prediction of microscopic structural instability may be obtained by an appropriate definition of macroscopic stability measure. This is in contrast with the classical macroscopic stability measure based on the strong ellipticity condition of the homogenized nominal moduli tensor, which gives unconservative estimations of the primary microscopic instability load except when the microscopic instability mode is global in nature.

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