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Microcracked materials as non-simple continua

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Abstract. A non-simple continuum model is adopted to grossly describe the behaviour of elastic microcracked bodies. The constitutive relations, obtained using a multiscale modelling based on the hypotheses of the classical molecular theory of elasticity, allow taking into account the microscopic features of the material. Referring to a one-dimensional microcracked bar, the possibility of the continuum to reveal the presence of internal heterogeneities is investigated.

Introduction

This work is based on the formulation of a continuum model with microstructure, for the study of the mechanical behaviour of complex materials. We call such a continuum model non-simple (multifield) continuum because of the presence of many field descriptors and of their gradients accounting for the material internal structure [1]. In particular, attention is focused on composite media made of short, stiff and strong fibres, having the same local rotation, embedded in a deformable matrix with a distribution of microcracks. These materials are modelled as continua with two independent kinematical field descriptors: the standard displacement field and one additional field accounting for the displacement jump occurring over the microcracks.

In analogy with the approach of the molecular theory of elasticity [2], such a model can been obtained by describing the mechanical behaviour of a complex lattice model (micromodel) and by linking different material scales (multiscale modelling) via an energy equivalence criterion [3]-[7].

In a general nonlinear context this kind of procedure can be articulated in the following steps:

1) Formulation of the discrete model.
2) Construction of the continuum model, in general non-simple:
    a. Kinematical assumptions on the virtual velocities → Virtual strain measure rates and Virtual Power of the continuum model.
    b. Virtual Power→ balance equations of the continuum model.
3) Extraction of the constitutive behaviour:
    a. Kinematical assumptions on the deformation fields → Strain measures and Elastic Energy of the continuum model.
    b. Elastic Energy→ Constitutive relations of the continuum model.

Step (2) allows obtaining the structure of the continuum model, encoded in the virtual power formula, starting from the discrete model. Step (3) allows extracting constitutive information from the discrete model.

In the particular case of a hyperelastic material the steps (2) and (3) can be switched and the former can be directly derived from the latter. Furthermore, for linear elastic models the two steps substantially coincides.

In particular, in [3] the context was non-linear and the attention was focused on the step (2). In [5] and [7] the context was linear elastic and the attention was focused on the step (3). In [6] the relevant dispersive wave propagation properties of the multifield model in [3] were investigated. A slightly different point of view was adopted in [4], where the continuum and the discrete models are directly formulated and the two models are linked together at the constitutive level.

In that case the procedure was:
1) Direct formulation of the continuum model.
2) Direct formulation of the discrete model.
4) Extraction of the constitutive behaviour.

In the present work we focus our attention on the structure of the continuum model, as a direct, autonomous, model, by following this last point of view. We first delineate a more general, non-linear, theoretical framework of the non-simple continuous model adopted to describe microcracked materials. Then, after recalling the equivalence procedure used to derive the continuum constitutive relations, we point out some peculiar features of the model with the aid of a one-dimensional example.

The continuum multifield model. Let us consider a body placed at a given time in the Euclidean region C and identify the body with this region. First of all we consider the list of kinematical descriptors, which defines a 'complete placement' for the body point X at any time t,

$$U(t,x)=\{\mathbf{p}(t,X),\mathbf{d}(t,X)\}. \qquad (1)$$

where the vector $\mathbf{p}$ is the standard placement (macro-field) and the vector $\mathbf{d}$ represents the smeared microcrack opening displacement (micro-field).

$$\dot{U}(t,p)=\{\dot{\mathbf{p}}(t,X),\dot{\mathbf{d}}(t,X)\}\,, \qquad (2)$$

is the list of the velocities associated with $\mathbf{p}$ and $\mathbf{d}$ (dot indicates the time derivative).
In order to account for local interactions only, we construct a multifield continuum theory in which both the zero and the first order terms of the macro and microfields appear. Then the inner power, P^i, is a linear functional of $\dot{\mathbf{p}}$, $\dot{\mathbf{d}}$ and of their gradients, while the outer power, P^o, is a linear functional of $\dot{\mathbf{p}}$, $\dot{\mathbf{d}}$:

$$P^i=\int_{\Omega}(\mathbf{s}\cdot\dot{\mathbf{p}}+\mathbf{S}\cdot\nabla\dot{\mathbf{p}}+\mathbf{z}\cdot\dot{\mathbf{d}}+\mathbf{Z}\cdot\nabla\dot{\mathbf{d}})\,dV\,, \qquad (3)$$
$$P^o=\int_{\Omega}\mathbf{b}\cdot\dot{\mathbf{p}}\,dV+\int_{\Omega}\mathbf{g}\cdot\dot{\mathbf{d}}\,dV+\int_{\partial\Omega}\mathbf{Sn}\cdot\dot{\mathbf{p}}\,dV+\int_{\partial\Omega}\mathbf{Zn}\cdot\dot{\mathbf{d}}\,dV\,,$$

both defined over a body-part $\Omega\subseteq C$, where $\mathbf{n}$ is the outward normal to $\partial\Omega$ and where the vectors $\mathbf{s}$, $\mathbf{z}$ and the tensors $\mathbf{S}$, $\mathbf{Z}$ are generalized stress fields, while the vectors $\mathbf{b}$ and $\mathbf{g}$ are the bulk external actions.
According to the axiomatic description in [8], [9], in order to derive the balance equations of such a continuum the inner power is required to coincide with the outer power for any field $\dot{\mathbf{p}}$, $\dot{\mathbf{d}}$.
By using the divergence theorem, the following balance laws can be obtained:

$$div\,\mathbf{S}+\mathbf{b}=\mathbf{0}\,,$$
$$div\,\mathbf{Z}-\mathbf{z}+\mathbf{g}=\mathbf{0}\,. \qquad (4)$$

By imposing the invariance of the inner virtual power under changes of observer, herein defined as

$$\tilde{U}(t,p)=\{\tilde{\mathbf{p}}(t,X),\tilde{\mathbf{d}}(t,p)\}=\{\tilde{\mathbf{p}}_o(t)+\tilde{\mathbf{Q}}(t)(\mathbf{p}(t,X)-\mathbf{p}_o(t)),\ \tilde{\mathbf{Q}}(t)\mathbf{d}(t,X)\}\,, \qquad (5)$$

where $\tilde{\mathbf{Q}}$ is a rotation tensor and $\tilde{\mathbf{p}}_o$ represents the translation of the frame, we obtain some general constitutive prescriptions for the generalized stresses and a reduced formula for the inner power. In fact, the effect of a change of observer on the velocities can be written:

$$\dot{\tilde{U}}(t,p)=\{\dot{\tilde{\mathbf{p}}}(t,X),\dot{\tilde{\mathbf{d}}}(t,X)\}=\{\tilde{\mathbf{W}}(t)(\tilde{\mathbf{p}}(t,X)-\tilde{\mathbf{p}}_o(t))+\tilde{\mathbf{Q}}(t)\dot{\mathbf{p}}(t,X),\ \tilde{\mathbf{W}}(t)\tilde{\mathbf{d}}(t,X)+\tilde{\mathbf{Q}}(t)\dot{\mathbf{d}}(t,X)\}\,, \tag{6}$$

where $\tilde{\mathbf{W}}=\dot{\tilde{\mathbf{Q}}}\tilde{\mathbf{Q}}^{\mathrm{T}}$. Then the power expended after the change of observer is:

$$\tilde{P}^{\,i}=\int_{\Omega}(\tilde{\mathbf{s}}\cdot\dot{\tilde{\mathbf{p}}}+\tilde{\mathbf{S}}\cdot\nabla\dot{\tilde{\mathbf{p}}}+\tilde{\mathbf{z}}\cdot\dot{\tilde{\mathbf{d}}}+\dot{\tilde{\mathbf{Z}}}\cdot\nabla\dot{\tilde{\mathbf{d}}})\,dV\,. \tag{7}$$

By assuming that the power expended must be invariant:

$$\tilde{P}^{\,i}=P^{\,i}\qquad\forall\,\mathrm{Q}\ \ \tilde{\mathbf{p}}_o(t),\tilde{\mathbf{Q}}(t)\,, \tag{8}$$

we obtain:

$$\begin{aligned}&\mathbf{s}=\mathbf{0}\,,\\&skw(\mathbf{S}\nabla\mathbf{p}^{\mathrm{T}}+\mathbf{z}\otimes\mathbf{d}+\mathbf{Z}\,\nabla\mathbf{d}^{\mathrm{T}})=\mathbf{0}\,,\end{aligned} \tag{9}$$

These equations restrict the possible constitutive prescriptions on the dynamical quantities, by linking the skew parts of **S**, **z, Z** one to each other, in such a way that we cannot independently choose constitutive prescriptions for each one of them. Eq. (9b) ensures that the local equilibrium of moments is satisfied.
For eliminating the redundancy of dynamical quantities we can, for example, express the first term as a function of the other two

$$skw(\mathbf{S}\nabla\mathbf{p}^{\mathrm{T}})=-skw(\mathbf{z}\otimes\mathbf{d}+\mathbf{Z}\,\nabla\mathbf{d}^{\mathrm{T}}). \tag{10}$$

and write a reduced formula for the inner power, which defines other strict strain measure rates

$$P^{\,i}=\int_{\Omega}[\mathbf{P}\cdot\dot{\mathbf{E}}+\mathbf{z}\cdot(\dot{\mathbf{d}}-\mathbf{W}\mathbf{d})+\mathbf{Z}\cdot(\nabla\dot{\mathbf{d}}-\mathbf{W}\nabla\mathbf{d})]\,dV\,, \tag{11}$$

where $\mathbf{P}=(\mathbf{S}\ \nabla\mathbf{p}^{\mathrm{T}}+\nabla\mathbf{p}\ \mathbf{S}^{\mathrm{T}})/2$ and $\dot{\mathbf{E}}=(\nabla\dot{\mathbf{p}}+\nabla\dot{\mathbf{p}})/2$. The reduced coupled balance equations become:

$$\begin{aligned}&div\,\mathbf{P}+div\,[\mathrm{skw}(\mathbf{z}\otimes\mathbf{d}+\mathbf{Z}\nabla\mathbf{d}^{\mathrm{T}})]+\mathbf{b}=\mathbf{0}\,,\\&div\,\mathbf{Z}-\mathbf{z}+\mathbf{g}=\mathbf{0}\,,\end{aligned} \tag{12}$$

where the only skew contribution in the first equation derives from the microstructure. This form of the balance equations involves only strict components of the generalized stress. In this way we can choose constitutive prescriptions for **P**, **z** and **Z** independently one from each other.
By linearizing the field equations near to the reference configuration we find:

$$\begin{aligned}&div\,\mathbf{T}+\mathbf{b}=\mathbf{0}\,,\\&div\,\mathbf{Z}-\mathbf{z}+\mathbf{g}=\mathbf{0}\,,\end{aligned} \tag{13}$$

where **T** is the Cauchy symmetric stress tensor. Then the inner power becomes

$$P^{\,i}=\int_{\Omega}(\mathbf{S}\bullet\dot{\mathbf{E}}+\mathbf{z}\bullet\dot{\mathbf{d}}+\mathbf{Z}\bullet\nabla\dot{\mathbf{d}})\,dV\,. \tag{14}$$

The constitutive model. At the microscopic level the reference microcracked material is described by two interacting lattice systems: one lattice made of interacting rigid particles of given shape,

representing the fibres and the other lattice made of interacting slits of arbitrary shape with a predominant dimension, representing the microcracks. The equivalence procedure which allows to identify the constitutive functions for the continuum internal actions by linking two different scale models is based on two hypotheses: (i) macroscopic homogeneous linearized deformations are imposed to a representative volume element (module) of the material periodic microstructure; (ii) the volume average of the power expended on the module is equated, through the localization theorem, to the inner power density of the macromodel. Briefly, the linearized strain measures of the module are: (a) the relative displacement between two points, $\mathbf{p}^a$ and $\mathbf{p}^b$, belonging to two particles A and B, represented by the vector $\mathbf{u}^{ab}$; (b) the relative rotation between A and B, represented by the skew-symmetric tensor $\mathbf{W}^{ab}$; (c) the opening-displacement at the centre of a slit H, represented by the vector $\mathbf{d}^h$; (d) the relative displacement between pair (H, K) of slits, $\mathbf{d}^h$ - $\mathbf{d}^k$; (e) the relative displacement between two points, $\mathbf{p}^a$ and $\mathbf{p}^h$, of a particle A and a slit H, also accounting for $\mathbf{d}^h$, represented by the vector $\boldsymbol{\omega}^{ah}$. The generalized forces associated with the above kinematical quantities are: (a) the force and (b) the couple between A and B, represented by the vector $\mathbf{t}^{ab}$ and the skew-symmetric tensor $\mathbf{C}^{ab}$, respectively; (c) the opening force on H, represented by the vector $\mathbf{z}^h$; (d) the slit interaction force between H and K, represented by the vector $\mathbf{z}^{hk}$; (e) the particle-slit interaction force, represented by the vector $\mathbf{q}^{ah}$.
The mean power of the module, of volume V, reads

$$\bar{P} = \frac{1}{V}\{\sum_{ab}[\mathbf{t}^{ab}\cdot(\dot{\mathbf{u}}^{ab} - \dot{\mathbf{W}}^{a}(\mathbf{p}^a - \mathbf{p}^b)) + \frac{1}{2}\mathbf{C}^{ab}\cdot(\dot{\mathbf{W}}^{ab})] + \sum_h \mathbf{z}^h\cdot\dot{\mathbf{d}}^h + \sum_{hk}\mathbf{z}^{hk}\cdot\dot{\mathbf{d}}^{hk} + \sum_{ah}\mathbf{q}^{ah}\cdot(\boldsymbol{\omega}^{ah} - \dot{\mathbf{W}}^a(\mathbf{p}^a - \mathbf{p}^h))\}. \tag{15}$$

where $\dot{\mathbf{W}}^a$ is the angular velocity of the reference particle A.
Based on hypothesis (i) all of the kinematical descriptors can be expressed in terms of regular fields defined on the current configuration of the multifield continuum, namely: the standard displacement vector field, $\mathbf{u}=\mathbf{p}-X$; the skew-symmetric part of the displacement gradient, $\mathbf{W}$; and the microdisplacement vector field, $\mathbf{d}$. The non-standard microscopic field account for the distributed displacement jump due to the presence of microcracks in the matrix. Then the power of the module becomes a function of the fields $\dot{\mathbf{E}}$, $\dot{\mathbf{d}}$ and $\nabla\dot{\mathbf{d}}$.
In this case a constrained lattice model, in which the particle rotations are assumed constant in the module, must be considered (Voigt's hypothesis [2], p. 599) and the internal power of the module reduces to

$$\bar{P} = \frac{1}{V}\{\sum_{ab}\mathbf{t}^{ab}\cdot\dot{\mathbf{u}}^{ab} + \sum_h \mathbf{z}^h\cdot\dot{\mathbf{d}}^h + \sum_{hk}\mathbf{z}^{hk}\cdot\dot{\mathbf{d}}^{hk}\} = \bar{P}(\dot{\mathbf{E}}, \dot{\mathbf{d}}, \nabla\dot{\mathbf{d}}). \tag{16}$$

Then, the power in Eq. (16) can be equated to the one in Eq. (14) for any $\dot{\mathbf{E}}$, $\dot{\mathbf{d}}$, $\nabla\dot{\mathbf{d}}$.
If, to a first approximation, all of the generalized forces are assumed linear elastic functions of the corresponding strain measures, after some algebraic manipulations, the stress-strain relations read

$$\begin{aligned} \mathbf{S} &= \mathsf{A}\,\mathbf{E} + \mathsf{C}\,\mathbf{d} + \mathsf{D}\,\nabla\mathbf{d}, \\ \mathbf{z} &= \mathsf{I}\,\mathbf{E} + \mathsf{M}\,\mathbf{d} + \mathsf{N}\,\nabla\mathbf{d}, \\ \mathbf{Z} &= \mathsf{O}\,\mathbf{E} + \mathsf{Q}\,\mathbf{d} + \mathsf{R}\,\nabla\mathbf{d}, \end{aligned} \tag{17}$$

where **A**, **C**, **D**, **I**, **M**, **N**, **O**, **Q**, **R** are elastic tensors of different order with components depending on the size, shape, arrangement and orientation of the internal phases, besides on the elastic constants of the matrix. In Eqs. (17) moreover, the material hyperelasticity entails symmetry relations between the components of the pairs of tensors (**C**, **I**), (**D**, **O**), (**N**, **Q**). If the material microstructure is arranged respecting the central symmetry, as in the case of any periodic microstructure, the tensors **C**, **I**, **N**, **Q** are null. In such circumstances the constitutive equations for the stress measures become

$$\begin{aligned} \mathbf{S} &= \mathbf{A}\ \nabla\mathbf{u} + \mathbf{D}\ \nabla\mathbf{d}, \\ \mathbf{z} &= \ \mathbf{M}\ \mathbf{d}, \\ \mathbf{Z} &= \mathbf{O}\ \nabla\mathbf{u} + \mathbf{R}\ \nabla\mathbf{d}. \end{aligned} \tag{18}$$

A one-dimensional problem. The reference system is a one-dimensional bar of length L=100cm, characterised by a uniform distribution of microcracks, of length l_m, arranged according to the transverse isotropic symmetry. Denoting with *u* and *d* the longitudinal components of the macrodisplacement and microdisplacement fields, respectively, the constitutive relations for the non null stress measures are

$$\begin{aligned} S &= \mathsf{A}\, u' + \mathsf{D}\ d', \\ z &= \mathsf{M}\, d, \\ Z &= \mathsf{O}\, u' + \mathsf{R}\ d'\ , \end{aligned} \tag{19}$$

where $\mathsf{A}, \mathsf{D}, \mathsf{M}, \mathsf{O}, \mathsf{R}$ are the sole independent components of the constitutive tensors in Eqs. (18) (apex indicates the spatial derivative). In particular for the considered system, A =Y, the Young's modulus; $\mathsf{R} = \mathrm{nY}/\rho_m\pi\ l_m$ and $\mathsf{M} = \mathrm{mY}\rho_m/\pi l_m$, where ρ_m is the microcrack density per unit length, and n and m are constants depending on the number and arrangement of the slits in the module [4]. The coupling term D=O, also depends on the microcrack size and arrangement and on the elastic constants of the matrix.
In the absence of body actions the Navier's equations read:

$$\begin{aligned} &\mathsf{A}\, u'' + \mathsf{D}\, d'' = 0\ , \\ &\mathsf{D}\, u'' + \mathsf{R}\, d'' - \mathsf{M}\, d = 0\ . \end{aligned} \tag{20}$$

We consider the constitutively uncoupled case, D=O=0. The bar is simply supported and subjected to a force F at the right end (*x*=L, being *x* the bar coordinate). In general, when traction on a microcracked bar is applied, this produces crack opening displacements that add to the standard displacement. Such a behaviour can be seen either as a consequence of the reduction of global stiffness (damage) or as an effect induced by an applied microforce. Herein, this latter viewpoint is adopted. Let us define the total displacement $u_t = u + d$ and assume the following macro and micro boundary conditions for this problem

$$\begin{aligned} &u_t(0) = u(0) + d(0) = 0 \\ &S(\mathrm{L}) = \mathrm{F}/\mathrm{A} \end{aligned} \quad \text{and} \quad Z(\mathrm{L}) = Z(-\mathrm{L}) = \lambda\, \mathrm{F}/\mathrm{A}\ , \tag{21}$$

where A is the cross sectional area of the bar and the applied microforce is assumed linearly depending on the applied macroforce, thorough a constant λ which can depend on material parameters of the microstructure. The solution in term of *u* is a standard linear solution $u(x) = (\mathrm{F}/\mathrm{YA})\, x - d(0)$, while the solution in terms of *d* is highly non-linear:

$$d(\mathrm{x}) = -\frac{F\lambda\, Sech[L\sqrt{\alpha}/2]\, Sinh[(L-2x)\sqrt{\alpha}/2]}{AY\sqrt{\alpha}} \tag{22}$$

where $\alpha = M/R = m/n\ \rho_m^2$.

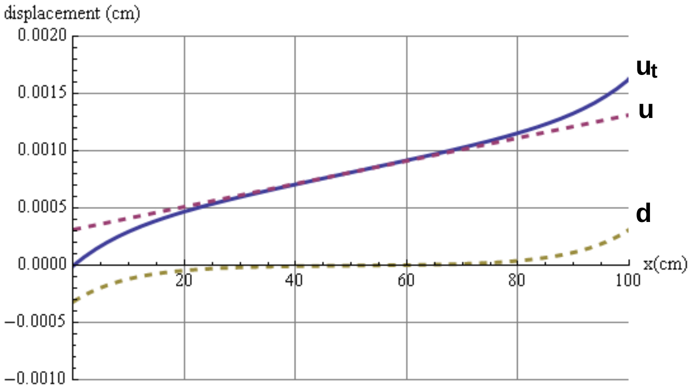

Fig. 1 Micro and macro displacement

Figure 1 shows the diagrams of the macrofield *u*, the microfield *d*, and the total displacement u_t vs the coordinate x, for a sample in which α=0.01 , $A=10^4 mm^2$, $Y=10^4\ N/mm^2$, $M=3.183x10^2\ N/mm^4$, $R=1.246x10^7\ N/mm^2$, $L=10^3$ mm, $F=10^3$ N, λ=π. The perturbation given by the microfield appears as a localized boundary effect, taking into account of the presence of the microcracks. The intensity of the perturbation and the localization depend on the microcrack density, through the material coefficients α and λ.

Final remarks

A continuum multifield description for microcracked elastic bodies equivalent to a lattice model has been proposed. The adopted multifield continuum model directly accounts for the presence and the spatial correlation between microcracks by means of additional kinematic and dynamic descriptors. This approach circumvents some theoretical problems related to the classical models with internal variables [10], [11]. The proposed model entails some difficulties related to the definition of the constitutive functions of all the dynamic quantities. Such problems have been tackled by an identification procedure based on an integral criterion of equivalence. The constitutive equivalent model is completely defined when the elastic constants and the geometry of the lattice model are known.

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