ARTICLE IN PRESS

Computers and Geotechnics xxx (xxxx) xxx–xxx

Contents lists available at ScienceDirect

Computers and Geotechnics

journal homepage: www.elsevier.com/locate/compgeo

Research Paper

Nonlocal enrichment of a micromechanical damage model with tensile softening: Advantages and limitations

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A R T I C L E I N F O

Keywords:
Continuum damage mechanics
Micromechanics
Anisotropic damage
Nonlocal regularization
Arc length control
Mixed mode fracture propagation

A B S T R A C T

Upon crack propagation, brittle geomaterials such as concrete and rock exhibit a nonlinear stress/strain behavior, damage induced stiffness anisotropy, loading path dependent strain softening and hardening, unilateral effects due to crack closure and a brittle-ductile transition, which depends on the confining pressure. Challenges in theoretical and numerical modeling include the distinction between tensile and compressive fracture propagation modes, mesh dependency during softening, and lack of convergence when several critical points are expected on the stress/strain curve. To overcome these issues, we formulate a nonlocal micromechanics based anisotropic damage model. A dilute homogenization scheme is adopted for calculating the deformation energy of the Representative Elementary Volume due to the displacement jumps at open and closed micro-cracks. Tension (respectively compression) damage criteria are expressed in terms of non-local equivalent strains defined in terms of positive principal strains (respectively deviatoric strains). Constitutive parameters are calibrated against published experimental data for concrete and shale. We employ the arc-length control method to solve boundary-value problems with the finite element package OOFEM: the algorithm allows capturing softening, snap back and snap through. We simulate the development of the compression damage zone around a cavity under various stress levels at the wall and far field, and the softening behavior consequent to tensile fracture propagation during a three-point bending test. No mesh dependency is noted during softening as long as micro-cracks do not interact.

1. Introduction

Understanding the mechanical behavior of quasi-brittle materials, such as concrete and rocks, is crucial in civil and petroleum engineering, for instance to analyze concrete structure failure or model hydraulic fracturing in reservoir rock. Laboratory experiments and field investigations show that the inception, growth and coalescence of micro cracks at the grain scale induce a complex nonlinear behavior at the macro-scale: tensile softening starts at a very low stress compared to the compressive yield stress, the formation of crack families of different orientations results in anisotropic stiffness reduction, crack closure produces unilateral effects, and in compression, a brittle-ductile transition occurs as the confining pressure is increased [1–4].

At the scale of a Representative Elementary Volume (REV - typically, the laboratory sample scale), Continuum Damage Mechanics (CDM) models are either based on phenomenology or micromechanics [5]. In phenomenological models, damage is an internal state variable defined as a tensor of second order [6–8] or fourth order [9,10], used to represent anisotropic stiffness reduction. The expression of energy potentials in terms of damage is constrained by symmetry and positivity requirements [11,12]. In order to satisfy thermodynamic consistency conditions, the energy release rate (damage driving force) that is work-conjugate to damage is used to construct damage criteria and damage potentials [13–15]. The inconvenient of phenomenological models is that the energy potentials are arbitrarily crafted to match observed stress/strain curves. As a result, constitutive relationships depend on material parameters that do not have any specific physical meaning. By contrast, in micromechanics, the material response at the REV scale is derived from matrix-inclusion interaction laws. Crack surface displacement jumps and local stresses are expressed explicitly and upscaled. Depending on whether the interaction among cracks is considered or not, a variety of homogenization techniques can be used, e.g. the dilute scheme [16–20], the self-consistent method [21–23], Mori-Tanaka scheme [24–26]. All of these models depend on the density of each crack family (i.e. each crack orientation). Cracks of a family are assumed to follow the same geometrical evolution laws, which are derived from fracture mechanics [27,28]. Under usual matrix-interaction assumptions, micro crack coalescence cannot be captured, which

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http://dx.doi.org/10.1016/j.compgeo.2017.09.011
Received 2 May 2017; Received in revised form 6 September 2017; Accepted 17 September 2017
0266-352X/

makes it impossible to model softening. In addition, most micromechanical approaches require the implementation of sophisticated iterative algorithms at the material point, which induces huge computational costs [29].

From a numerical perspective, simulation results become mesh-dependent when a local softening constitutive model is used to analyze failure. Strain localization renders the problem mathematically ill-posed [30,31]. The regularization techniques that are the most widely used to address this issue are differentiation based and integration based nonlocal formulations. Differentiation-based models are enriched with the first or higher-order gradient of state variables or thermodynamic forces, which allows accounting for the variations of variables within a neighborhood around material points [32–35]. When the gradients of state variables are used in the formulation, additional degrees of freedom need to be implemented for Finite Element Analysis, for instance the third-order stress tensor (conjugate to the gradient of deformation). In integration based nonlocal models, a variable at a point is calculated as a weighted average over a certain neighborhood of that point [36–40]. The weights that quantify the intensity of the interaction between Gauss points is tabulated, so that each Gauss point interacts with the Gauss points in its neighborhood. The size of the neighborhood is determined by an internal length parameter. Advantages and limitations of the different regularization techniques are discussed in [41]. Another challenge of failure analysis is non-convergence issues encountered at the global iteration level. The classical Newton-Raphson scheme based on loading control only or displacement control only works when only hardening effects are considered. In case of snap back or snap through, more advanced methods, such as line search [42] or arc length control [43,44] need to be used.

In this paper, we derive the expression of damage energy potentials from micromechanics to formulate and implement a nonlocal anisotropic damage model. Under the assumption of crack non-interaction, the free enthalpy is obtained by integrating open and closed crack surface displacement jumps in all possible crack orientations within a unit sphere (Section 2). We construct equivalent strains induced by open and closed cracks. Following a phenomenological approach, we formulate two damage criteria and two damage potentials to predict the evolution of crack density. Single element simulations (at the Gauss point) of cyclic uniaxial tension-compression and triaxial compression tests demonstrate the capabilities of the proposed framework. In Section 3, we explain the theory and implementation of the nonlocal model and we describe the arc length control method employed in the resolution algorithm. In Section 4, we calibrate the proposed damage model against published experimental results of triaxial compression tests performed on shale and uniaxial tension tests performed on concrete. We simulate damage development around a circular cavity, with an initial confining pressure followed by different stress paths. We also simulate a three-point bending test with the calibrated model parameters.

2. Local anisotropic damage model

2.1. Micromechanics-based Gibbs energy

We adopt the expression of the free enthalpy established in [45], for a REV of volume Ω_r and external boundary $\partial\Omega_r$ subjected to a uniform stress $\boldsymbol{\sigma}$. It is assumed that a large number of penny shaped microscopic cracks of various orientations are embedded in an isotropic linear elastic matrix of compliance tensor $\mathbb{S}_0$. Each microscopic crack is characterized by its normal direction $\vec{n}$ and its radius a, which is at least 100 times smaller than the REV size. Opposite crack faces are noted ω^+ and ω^-, with normal vectors $\vec{n}^+$ and $\vec{n}^-$. The macro strain of a REV that contains a single set of N microcrack oriented in planes normal to $\vec{n}$ is the sum of the elastic strains of the matrix and the strains due to the normal and shear crack displacement jumps, denoted as $[u_n]$ and $[\vec{u_t}]$ respectively. Therefore:

$$\epsilon = \mathbb{S}_0: \boldsymbol{\sigma} + \frac{N}{|\Omega_r|}\int_{\partial\omega^+}[u_n](\vec{n}\otimes\vec{n})\mathrm{d}S + \frac{N}{2|\Omega_r|}\int_{\partial\omega^+}([\vec{u_t}]\otimes\vec{n} + \vec{n}\otimes[\vec{u_t}])\mathrm{d}S \tag{1}$$

Since it is assumed that cracks do not interact, we use a dilute homogenization scheme. The stress that acts on crack faces is a direct projection of the macroscopic stress (i.e. stress at the REV scale). According to fracture mechanics principles, the average normal and shear displacement jumps for a single crack embedded in a linear isotropic elastic matrix can be expressed as follows [21,46,47]:

$$\langle[u_n]\rangle = \frac{16}{3}\frac{1-\nu_0^2}{\pi E_0}\boldsymbol{\sigma}:(\vec{n}\otimes\vec{n})a$$
$$\langle[\vec{u_t}]\rangle = \frac{32}{3}\frac{1-\nu_0^2}{(2-\nu_0)\pi E_0}[\boldsymbol{\sigma}\cdot\vec{n_i} - (\vec{n}\cdot\boldsymbol{\sigma}\cdot\vec{n})\vec{n}]a \tag{2}$$

In which E_0 and ν_0 are the Young's modulus and Poisson's ratio of the matrix, respectively.

Correspondingly, the average volume fraction of the normal and shear displacement jumps for a single family of cracks are calculated as:

$$\beta = \frac{N}{|\Omega_r|}\langle[u_n]\rangle\pi a^2, \quad \vec{\gamma} = \frac{N}{|\Omega_r|}\langle[\vec{u_t}]\rangle\pi a^2 \tag{3}$$

The elastic free enthalpy of the cracked REV can be expressed as

$$G^* = \frac{1}{2}\boldsymbol{\sigma}:\epsilon = \frac{1}{2}\boldsymbol{\sigma}:\mathbb{S}_0:\boldsymbol{\sigma} + \frac{1}{2}\boldsymbol{\sigma}:[\beta\vec{n}\otimes\vec{n} + \frac{1}{2}(\vec{\gamma}\otimes\vec{n} + \vec{n}\otimes\vec{\gamma})] \tag{4}$$

A normal displacement jump can only be induced by a tensile force, i.e. for $\vec{n}\cdot\boldsymbol{\sigma}\cdot\vec{n} \geqslant 0$. The unilateral contact condition at crack faces can thus be expressed as:

$$[u_n] \geqslant 0, \quad \sigma_{nn} = \vec{n}\cdot\boldsymbol{\sigma}\cdot\vec{n} \geqslant 0, \quad [u_n]\sigma_{nn} = 0 \tag{5}$$

After combining all the equations above, the free enthalpy for the considered REV with a single set of N cracks is expressed as:

$$G^* = \frac{1}{2}\boldsymbol{\sigma}:\mathbb{S}_0:\boldsymbol{\sigma} + \frac{1}{2}c_0\rho(\vec{n}\cdot\boldsymbol{\sigma}\cdot\vec{n})\langle\vec{n}\cdot\boldsymbol{\sigma}\cdot\vec{n}\rangle + \frac{1}{2}c_1\rho[(\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}):(\vec{n}\otimes\vec{n}) - \boldsymbol{\sigma}:(\vec{n}\otimes\vec{n}\otimes\vec{n}\otimes\vec{n}):\boldsymbol{\sigma}] \tag{6}$$

In which we note $\langle x\rangle^+ = x, x \geqslant 0$, and $\langle x\rangle^+ = 0, x < 0$. The coefficient c_0 (respectively c_1) is defined as the normal (respectively shear) elastic compliance of the crack. $\rho(\vec{n})$ is the crack density, for the set of N cracks oriented in planes perpendicular to $\vec{n}$. We define:

$$c_0 = \frac{16}{3}\frac{1-\nu_0^2}{E_0}, \quad c_1 = \frac{32}{3}\frac{1-\nu_0^2}{(2-\nu_0)E_0}, \quad \rho = \frac{Na^3}{|\Omega_r|} \tag{7}$$

For several crack sets of different orientations, the Gibbs free energy of the REV is obtained by integrating G^* for a distribution of crack densities $\rho(\vec{n})$, over the unit sphere $S^2 = \{\vec{n}, |\vec{n}| = 1\}$, as follows:

$$G = \frac{1}{2}\boldsymbol{\sigma}:\mathbb{S}_0:\boldsymbol{\sigma} + \frac{1}{8\pi}\int_{S^2}\{c_0\rho(\vec{n})(\vec{n}\cdot\boldsymbol{\sigma}\cdot\vec{n})\langle\vec{n}\cdot\boldsymbol{\sigma}\cdot\vec{n}\rangle + c_1\rho(\vec{n})[(\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}):(\vec{n}\otimes\vec{n}) - \boldsymbol{\sigma}:(\vec{n}\otimes\vec{n}\otimes\vec{n}\otimes\vec{n}):\boldsymbol{\sigma}]\}\mathrm{d}S \tag{8}$$

At the scale of the REV, the second order crack density tensor $\boldsymbol{\rho}$ is defined in such a way that: $\rho(\vec{n}) = \vec{n}\cdot\boldsymbol{\rho}\cdot\vec{n}$. The second order damage tensor is defined as follows:

$$\boldsymbol{\Omega} = \frac{1}{4\pi}\int_{S^2}\rho(\vec{n})(\vec{n}\otimes\vec{n})\mathrm{d}S = \frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi}\rho(\vec{n})(\vec{n}\otimes\vec{n})sin\theta\mathrm{d}\phi\mathrm{d}\theta \tag{9}$$

It can be shown mathematically (see [48,49] for details) that the crack density function $\rho(\vec{n})$ is related to the damage tensor as follows:

$$\rho(\vec{n}) = \frac{3}{2}(5\vec{n}\cdot\boldsymbol{\Omega}\cdot\vec{n} - \mathrm{Tr}\boldsymbol{\Omega}) \tag{10}$$

The free energy is the sum of the elastic deformation energy stored in the matrix and the elastic energy stored by displacement jumps across