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Modelling of microcracking in image-based models of highly heterogeneous materials using the phase field method

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Micro Abstract
Crack nucleation and propagation in heterogeneous materials models, as obtained by X-Ray micro-CT imagery, is investigated by the phase field method. Several 3D analyses in highly heterogeneous materials are carried out, with application to cementitious materials. Direct comparisons of complex 3D micro cracking in heterogeneous quasi-brittle materials modeled by the phase field numerical method and observed by imaging during in situ mechanical testing are presented.

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Introduction

Predicting the strength due to cracking in quasi-brittle materials such as concrete or other civil engineering materials is of formidable interest. Crack propagation modelling in brittle or quasi-brittle materials has long been restricted to simple academic cases and to the macroscopic scale. With recent advances in both numerical simulation methods and experimental characterization, new studies are now possible, allowing the development of fracture models at microscale, in particular from realistic microstructure morphologies of complex materials such as concrete. However, developing predictive models of crack initiation and propagation in three-dimensional complex heterogeneous microstructures is still highly challenging regarding modelling, numerical simulation methods, and experimental characterization.

In the present work, we precisely aim at tackling the difficult issue of developing a predictive model for 3D crack propagation in heterogeneous quasi-brittle materials microstructures. A phase field method based on the variational formulation of the crack evolution problem [3] and its numerical implementation as proposed by [4] is used to simulate crack initiation and propagation in realistic microstructure models obtained by XR-μCT. Then, *in situ* testing combined with XR-μCT is carried out to experimentally follow the 3D crack paths by means of a specific image subtraction procedure using Digital Volume Correlation (DVC). Direct comparisons between the numerical model simulations of crack paths and experimental data are performed. In addition, some parameters of the constitutive relation of the quasi-brittle material model are identified by inverse analysis combining experiments and simulations [5].

1 Brief recall of phase field damage model

In the following, the basic concepts of the phase field method are briefly summarized. For more details and practical implementation aspects, the interested reader can refer to [4,7]. The phase field method is based on a regularized formulation of a sharp crack description. A regularized variational principle describes both the evolution of the mechanical problem and of an additional field d describing the damage (called phase field). It is discretized by a finite element procedure and a staggered algorithm, chosen here due to its numerical efficiency. As compared to classical volume damage models, such regularized approach is directly connected to the theory of brittle crack propagation and removes mesh-sensitivity issues due to its natural nonlocal character.

In the phase field method, assuming small strains, the regularized form of the energy describing the cracked structure is expressed by:

$$E(\mathbf{u}, d) = \int_{\Omega} W(\mathbf{u}, d) d\Omega + g_c \int_{\Omega} \gamma(d, \nabla d) d\Omega, \tag{1}$$

where W is the density of the elastic energy, depending on the displacements $\mathbf{u}(\mathbf{x})$ and on the phase field $d(\mathbf{x})$ describing the damage of the solid, g_c is the fracture resistance and $\gamma(d, \nabla d)$ is the crack energy density, defined by $\gamma(d, \nabla d) = \frac{1}{2\ell} d^2 + \frac{l}{2} \nabla d \cdot \nabla d$ (see e.g. [4, 7]). Applying the principle of maximum dissipation and energy minimization [3] to (1) yields the set of coupled equations to be solved on the domain Ω associated with the structure, with boundary $\partial\Omega$ and outward normal $\mathbf{n}$, to determine $d(\mathbf{x})$ and $\mathbf{u}(\mathbf{x})$, $\forall \mathbf{x} \in \Omega$:

$$\begin{cases} 2(1-d)\mathcal{H} - \frac{g_c}{\ell} \left\{ d - \ell^2 \Delta d \right\} = 0 \quad \text{in } \Omega, \\ d(\mathbf{x}) = 1 \quad \text{on } \Gamma, \\ \nabla d(\mathbf{x}) \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega, \end{cases} \tag{2}$$

and

$$\begin{cases} \nabla \cdot \boldsymbol{\sigma}(\mathbf{u}, d) = \mathbf{f} \quad \text{in } \Omega, \\ \mathbf{u}(\mathbf{x}) = \overline{\mathbf{u}} \quad \text{on } \partial\Omega_u, \\ \boldsymbol{\sigma}\mathbf{n} = \overline{\mathbf{F}} \quad \text{on } \partial\Omega_F. \end{cases} \tag{3}$$

In (2), Γ refers to the crack surface, ℓ is the regularization parameter. The history strain energy density function $\mathcal{H}(\mathbf{x}, t)$, where t denotes time, is introduced to describe a dependence on history [4] and possible loading-unloading, and reads:

$$\mathcal{H}(\mathbf{x}, t) = \underset{\tau \in [0,t]}{max} \left\{ \Psi^+ (\mathbf{x}, \tau) \right\}. \tag{4}$$

In (4), Ψ^+ is the tensile part of the elastic strain density function serving to model unilateral contact, and is defined as

$$\Psi^+(\boldsymbol{\varepsilon}) = \frac{\lambda}{2} \left(\langle Tr(\boldsymbol{\varepsilon}) \rangle_+ \right)^2 + \mu Tr \left\{ \left(\boldsymbol{\varepsilon}^+ \right)^2 \right\}, \tag{5}$$

where $\boldsymbol{\varepsilon}$ is the linearized strain tensor, $\langle x \rangle_{\pm} = (x \pm |x|)/2$ and $\boldsymbol{\varepsilon}^{\pm}$ are compression and tensile parts of the strain tensor (see e.g. [4, 7]). The choice of the numerical parameter ℓ has been discussed e.g. in [1, 2, 6, 8].

2 Illustrative example

We provide in this section an illustrative example of the present framework. A sample of lightweight concrete, i.e. a concrete embedding light inclusions (EPS beads and small pores), is investigated. Such case is challenging, as the microstructure cannot be easily idealized by basic shapes (see Fig. 2). The material is composed of three phases: the sand grains, the plaster matrix, and the pores. Here, the whole segmented image of the sample involves several billions of voxels. To make the problem tractable and to allow the use of a mapping of voxels properties to a regular mesh of elements, we adopt here a sub-volume technique, described in [5], where the displacements identified by 3D image correlation during an in-situ experiment are prescribed on the boundary of a sub-volume of size $240 \times 240 \times 64$ voxel^{3}cut in the sample (see Fig. 1). The obtained mesh is composed of 3.7 million of regular 8-node elements. In Fig. 2 We compare the crack propagation obtained by experiment and numerical simulation for the same load loading. The obtained results are in very good agreement with the experimentally observed 3D crack path. Other applications and extensions from the recent works by the authors [5–7] will be presented.

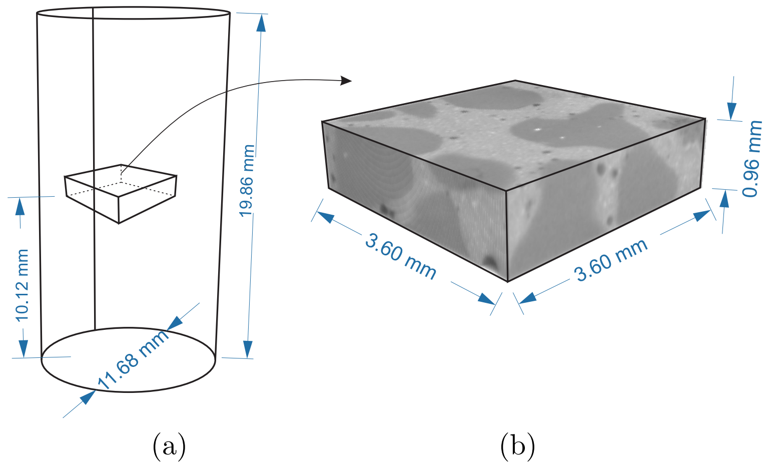

Figure 1. Geometry of a sub-volume of lightweight concrete: (a) location in the sample; (b) XR-μCT images of the sub-volume.

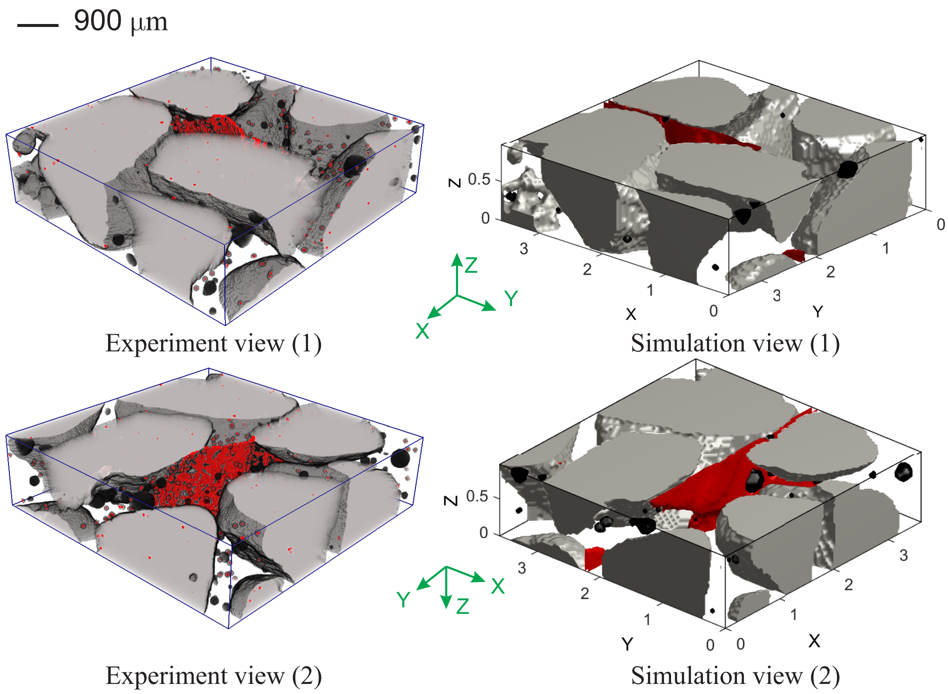

Figure 2. Comparison between experimental crack obtained from microtomography and from phase field method of the lightweight concrete sample in the studied sub-volume for a load $F = 1.8$ kN. (Left: experiment; right: numerical simulation.)

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References

[1] H. Amor, J.-J. Marigo, and C. Maurini. Regularized formulation of the variational brittle fracture with unilateral contact: Numerical experiments. *J. Mech. Phys. Solids*, 57(8):1209–1229, 2009.

[2] M. Borden, C. Verhoosel, M. Scott, T. Hughes, and C. Landis. A phase-field description of dynamic brittle fracture. *Comput. Meth. Appl. Mech. Eng.*, 217:77–95, 2012.

[3] G. Francfort and J. Marigo. Revisiting brittle fracture as an energy minimization problem. *J. Mech. Phys. Solids*, 46(8):1319–1342, 1998.

[4] C. Miehe, M. Hofacker, and F. Welschinger. A phase field model for rate-independent crack propagation: Robust algorithmic implementation based on operator splits. *Comput. Meth. Appl. Mech. Eng.*, 199:2776–2778, 2010.

[5] T. Nguyen, J. Yvonnet, M. Bornert, and C. Chateau. Direct comparisons of 3D crack networks propagation in cementitious materials between phase field numerical modeling and in-situ microtomography experimental images. *J. Mech. Phys. Solids*, 95:320–350, 2016.

[6] T. Nguyen, J. Yvonnet, M. Bornert, C. Chateau, K. Sab, R. Romani, and R. L. Roy. On the choice of parameters in the phase field method for simulating crack initiation with experimental validation. *Int. J. Fract.*, 197(2):213–226, 2016.

[7] T. Nguyen, J. Yvonnet, Q.-Z. Zhu, M. Bornert, and C. Chateau. A phase field method to simulate crack nucleation and propagation in strongly heterogeneous materials from direct imaging of their microstructure. *Eng. Frac. Mech.*, 139:18–39, 2015.

[8] K. Pham, J.-J. Marigo, and C. Maurini. The issues of the uniqueness and the stability of the homogeneous response in uniaxial tests with gradient damage models. *J. Mech. Phys. Solids*, (6), 2011.