Morphogenesis and propagation of complex cracks induced by thermal shocks
Supplementary Material

Blaise Bourdin,[1] Jean-Jacques Marigo,[2] Corrado Maurini,[3,4] and Paul Sicsic[2,5]

[1] *Department of Mathematics and Center for Computation & Technology, Louisiana State University, Baton Rouge, LA 70803, USA*
[2] *Laboratoire de Mécanique des Solides (UMR-CNRS 7649), École Polytechnique, 91128 Palaiseau Cedex*
[3] *Université Paris 6 (UPMC), 4 place Jussieu, 75252 Paris, France*
[4] *Institut Jean Le Rond d'Alembert (UMR-CNRS 7190), 4 place Jussieu, 75252 Paris, France*
[5] *Lafarge Centre de Recherche, 95 Rue de Montmurier 38290 St-Quentin-Fallavier, France*

(Dated: September 12, 2013)

GRADIENT DAMAGE MODEL.

Formulation

The total energy we consider is a variant of the regularized energy introduced in [3], fitting within the broader class considered in [4]:

$$\mathcal{E}_t(u,\alpha) = \int_\Omega \frac{\psi_t(\varepsilon)}{s(\alpha)} + \frac{G_c}{4c_w}\left(\frac{w(\alpha)}{\ell} + \ell\,|\nabla\alpha|^2\right)\mathrm{d}x. \tag{1}$$

The convergence analysis requires the addition of a small *residual stiffness* associated to a fully damaged state. It is now well established that the addition of this parameter has no significant impact on numerical simulation, so it has been omitted throughout the article. The quasi-static evolution problem for the displacement and the damage field follows the formulation in [10] and fits within the framework of rate-independent processes [8]. At each time t, $(u_t,\, \alpha_t)$ satisfies the following three conditions: *(i) Irreversibility*: the damage field is a non-decreasing function of time. *(ii) Unilateral stability*: the displacement and damage fields are local minimizers of the total energy amongst all kinematically admissible displacements and all damage fields satisfying the irreversibility condition. *(iii) Energy balance:* the variation of the total energy is equal to the work of the external loadings. Condition *(i)* forbids healing and condition *(ii)* implies equilibrium equation (energy minimality with respect to u) and the damage criterion (bound-constrained minimality with respect to α), defining a *elastic domain*

$$\frac{s'(\alpha)\psi_t(\varepsilon)}{s^2(\alpha)} \le \frac{G_c}{4c_w}\left(\frac{w'(\alpha)}{\ell} - 2\ell\,\nabla^2\alpha\right), \tag{2}$$

where ∇^2 stands for the Laplacian. Finally condition *(iii)* leads to the consistency condition

$$\left(\frac{s'(\alpha)\psi_t(\varepsilon)}{s^2(\alpha)} - \frac{G_c}{4c_w}\left(\frac{w'(\alpha)}{\ell} - 2\ell\,\nabla^2\alpha\right)\right)\dot\alpha = 0. \tag{3}$$

which enforces that damage can only evolve when the material is on the boundary of the elastic domain. Accounting for the constitutive relation for linear thermo-elasticity $\varepsilon - \varepsilon^{\mathrm{th}} = s(\alpha)A_0^{-1}\sigma$, on obtains that

$$\frac{\psi_t(\varepsilon)}{s^2(\alpha)} = \frac{1}{2\,s^2(\alpha)}\mathsf{A}_0(\varepsilon-\varepsilon^{\mathrm{th}})^2 = \frac{1}{2}\mathsf{A}_0^{-1}\sigma^2$$

Hence, for homogenous damage distribution such that $\nabla^2\alpha = 0$, equation (2) may be written in the form

$$\mathsf{A}_0^{-1}\sigma^2 \le \frac{G_c}{2c_w\ell}\frac{w'(\alpha)}{s'(\alpha)}, \tag{4}$$

showing that the domain of admissible stresses depends on $w'(\alpha)/s'(\alpha)$. If $w'(\alpha)/s'(\alpha)$ is an increasing (resp. decreasing) function of α, the material is said to be *stress hardening* (resp. *stress softening*).

Moreover at $\alpha = 0$ and for uniaxial stress states, equation (4) reads as:

$$\sigma \le \sigma_{\mathsf{c}} = \sqrt{\frac{G_c E}{2c_w\ell}\frac{w'(0)}{s'(0)}}, \tag{5}$$

which gives the expression for the elastic limit reported in equation (3) of the article.

Constraints on energy dictated by thermodynamical and mechanical consistency

Mechanical and thermodynamical consistency impose certain conditions on $s(\alpha)$, $w(\alpha)$ (see the complete discussion in [11]). In order for the total energy (1) to be a valid approximation of a Griffith-like fracture energy, when the damage variable α reaches its maximal value 1 the residual stress must vanish, and the dissipated energy to reach that state should be finite. Moreover, $s(\alpha)$ must be non-negative (positive elasticity), monotonically increasing (decreasing stiffness) with $s(0) = 1$ and $\lim_{\alpha\to 1} s(\alpha) = \infty$; $w(\alpha)$ must be positive and monotonically increasing (positive dissipation) with $\int_0^1 \sqrt{w(\alpha)} < \infty$; $w'(\alpha)/s'(\alpha)$ must monotonically decrease to 0, at least for α close to 1 (stress-softening). This condition can be weakened by requiring stress-softening only in subset $(\alpha_0, 1]$. Indeed, it is not respected for α close to 0 for the models of [3].

Under these hypotheses, it is known (see [4] for instance) that the global minimizers of (1) approach that of the Griffith–like energy $\int_{\Omega\setminus\Gamma} \psi_t(\varepsilon)\,\mathrm{d}\mathbf{x} + G_c\mathcal{S}(\Gamma)$, where $\mathcal{S}$ is the surface measure of the cracks Γ, and $c_w = \int_0^1 \sqrt{w(\alpha)}\,\mathrm{d}\alpha$. Furthermore using only the weaker conditions *(i)-(iii)* [13] have proven that damage band follow Griffith's evolution law, thus overcoming the global minimization. A similar result has been obtained for phase-field models in [6, 7].

In this letter, we use

$$s(\alpha) = 1/(1-\alpha)^2 \text{ and } w(\alpha) = \alpha. \tag{6}$$

The choice of this specific model is motivated by the existence of a critical stress, the finite dissipate energy to reach no residual stress and by its simplicity: the energy is quadratic with respect to u and α separately.

Identification of the internal length.

Additional informations on s and w can be obtained from the analysis of a uniaxial tension experiment [9, 11]. Stability analysis in the aforementioned references reveals that the sample remains damage-free as long as the stress field remains below the critical value σ_c, given by (5). For the specific choices of s and w used in this paper, we have

$$\sigma_{\mathsf{c}} = \sqrt{\frac{3G_cE}{8\ell}}. \tag{7}$$

Equation (7) allows for the identification of the internal length ℓ from the experimental measurements of the critical stress σ_c, the fracture toughness G_c, and the Young modules E. In doing so, we postulate that the internal length identified in the uniaxial experiment is relevant to other situations.

Localized solutions.

Solutions with localized damaged are the smeared representation of cracks. For the uniaxial traction test they have been constructed analytically in [9]. Using the damage criterion (2) and the energy balance (3), localized damage contained in a region $(x_i - L_\sigma,\, x_i + L_\sigma)$ must evolve in such a way that at each point,

$$s'(\alpha)\sigma^2 - \frac{G_c}{2c_w}\left(\frac{w'(\alpha)}{\ell} - 2\ell\,\alpha''\right) = 0, \tag{8}$$

where α'' denotes the spatial second derivative. Continuity of the damage field and its spatial derivative imposes that $\alpha(x_i \pm L_\sigma) = \alpha'(x_i \pm L_\sigma) = 0$ when the damage localizes from an elastic state $\alpha_0 = 0$. Integrating (8) with respect to x and using the boundary conditions in α one gets the first integral:

$$(s(\alpha) - 1)\sigma^2 - \frac{G_c}{2c_w}\left(\frac{w(\alpha)}{\ell} - \ell\,\alpha'^2\right) = 0, \tag{9}$$

which allows the construction of localization profile for any value of the stress σ by integrating a first order differential equation for which existence of solution is guaranteed if the material is stress-softening and $\sigma < \sigma_{\mathsf{c}}$. Cracks are viewed as localized damage zones with zero stress. In the limit $\sigma \to 0$, under the assumed constitutive hypothesis, (9) gives:

$$w(\alpha) = \ell^2\,\alpha'^2 \tag{10}$$

Hence, one can easily deduce the following expressions for the localization profile and the width of the localization band:

$$\alpha(x) = \left(1 - \frac{|x - x_i|}{2\ell}\right)^2, \qquad L_0 = 2\ell$$

Moreover, using (10) and performing a change of variable $x \to \alpha$, one can show that the energy dissipated in a single localization is

$$\frac{G_c}{4c_w}\int_{x_i - L_0/2}^{x_i + L_0/2}\left(\frac{w(\alpha)}{\ell} + \ell\ \alpha'^2\right)\mathrm{d}x = \frac{G_c}{c_w}\int_0^1 \sqrt{w(a)}d\alpha = G_c,$$

The equation above establishes a precise energetic equivalence between a single localization and a crack at fixed $\ell > 0$, and explains the rationale for the choice of the constant $c_w := \int_0^1 \sqrt{w(a)}d\alpha$. This one-dimensional study also provides informations on the shape and the properties of the damage profile for two- and three-dimensional cracks (see [11]).

NUMERICAL IMPLEMENTATION

The numerical implementation of this model is now classical and described in details in [1–3]. Irreversibility and unilateral stability are combined into a series of time discrete constrained minimization problems

$$\min_{u, \alpha \geq \alpha_{i-1}} \mathcal{E}_t(u, \alpha)$$

at time t_i, assuming the knowledge of the damage field at the previous time step t_{i-1}. The temperature field is obtained by solving the transient heat equation on the un-cracked domain using finite elements of using a close form solution when available. At each time step, the total energy is iteratively minimized with respect to the kinematically admissible displacement fields and damage fields satisfying an irreversibility constraint, a process known to converge to a pair $(u,\ \alpha)$ satisfying a time–discrete version of irreversibility and unilateral stationarity. Minimality with respect to the displacement field is equivalent to solving for static equilibrium while for the specific choice of w and s given above, unilateral minimality with respect to the damage field is a box-constraint minimization problem of a convex functional. The main difference with [3] is that at each discrete time step, irreversibility is accounted for as a constraint on the admissible damage fields.

POST-PROCESSING OF THE NUMERICAL RESULTS FOR THE SCALING LAWS IN FIG. 1,5

In the results of FIG. 1, the data associated with the numerical experiment is obtained through a specify automatized post-processing script counting the peaks of α on lines parallel to and at distance a from the edge of the domain, and experimental data are taken from [12]. Where cracks are revealed by a blue dye penetrating the cracks by capilarity then manually counted. In this procedure, capillary effects may prevent the detection of short crack with very small crack openings. In both case the analysis was limited to a central region of the slab, in order to avoid boundary effects.

For the scaling properties of three dimensional numerical simulation of FIG.5, the scaling properties of the fracture system are obtained using the following procedure. On a cross section parallel to the surface exposed to the thermal shock, the area of each of the connected component of the region $\alpha < .95$ is measured, discarding the ones in contact wit the lateral boundaries of the domain. This post-processing is performed using the VisIt visualization software [5].

[1] B. Bourdin. Numerical implementation of the variational formulation for quasi-static brittle fracture. *Interface Free Bound.*, 9:411—430, 2007.
[2] B. Bourdin, G-A. Francfort, and J-J. Marigo. The variational approach to fracture. *J. Elasticity*, 91:5–148, 2008.
[3] B. Bourdin, G.A. Francfort, and J-J. Marigo. Numerical experiments in revisited brittle fracture. *J. Mech. Phys. Solids*, 48(4):797 – 826, 2000.
[4] A. Braides. *Approximation of Free-Discontinuity Problems.* Lecture notes in Mathematics, vol. **1694**. Springer, 1998.

[5] H. Childs, E. S. Brugger, K. S. Bonnell, J. S. Meredith, M. Miller, B. J. Whitlock, and N. Max. A contract-based system for large data visualization. In *Proceedings of IEEE Visualization 2005*, pages 190–198, 2005.

[6] V. Hakim and A. Karma. Crack path prediction in anisotropic brittle materials. *Phys. Rev. Lett.*, 95:235501, Dec 2005.

[7] V. Hakim and A. Karma. Laws of crack motion and phase-field models of fracture. *J. Mech. Phys. Solids*, 57(2):342 – 368, 2009.

[8] A. Mielke. Evolution of rate-independent systems. In *Handbook of differential equations: Evolutionary Differential Equations*, volume II, pages 461–559. North-Holland, Amsterdam, 2005.

[9] K. Pham, H. Amor, J.-J. Marigo, and C. Maurini. Gradient damage models and their use to approximate brittle fracture. *Int. J. Damage Mech.*, 20(4):618–652, 2011.

[10] K. Pham and J.-J. Marigo. Approche variationnelle de l'endommagement : II. les modèles à gradient. *CR Mécanique*, 338(4):199–206, 2010.

[11] K. Pham and J.-J. Marigo. From the onset of damage up to the rupture: construction of the responses with damage localization for a general class of gradient damage models. *Continuum Mech. Thermodyn.*, 25(2-4):147–171, 2013.

[12] Y. Shao, Y. Zhang, X. Xu, Z. Zhou, W. Li, and B. Liu. Effect of crack pattern on the residual strength of ceramics after quenching. *J. Am. Ceram. Soc.*, 94(9):2804–2807, 2011.

[13] P. Sicsic and J.-J. Marigo. From gradient damage laws to Griffith's theory of crack propagation. To appear in *J. Elast*, 2012.