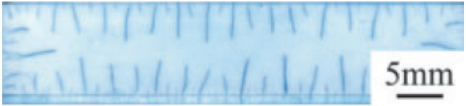
Nucleation of cracks and influence of defects in variational phase-field models of brittle fracture

C. Maurini[1], B. Bourdin[2], T. Li[3,4], J.-J. Marigo[3], E. Tanné[2,3]

[1] Institut Jean Le Rond d'Alembert, Université Pierre et Marie Curie and CNRS
[2] Department of Mathematics, Louisiana State University, US
[3] LMS, Ecole Polytechnique
[4]LAMSID, EDF R&D

28/11/2017, GDR Mephy, ESPCI-Paris

Fracture mechanics: complex examples



Thermal shock in ceramics (Song et al. 2011)

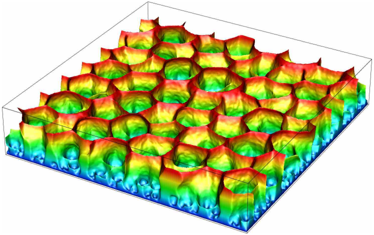
Thin film cracks

Giant's Causeway

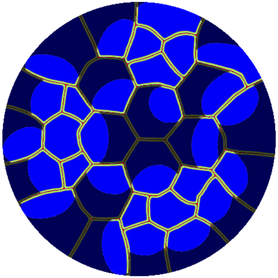
Modelling issues:

- Crack nucleation
- Morphogenesis of complex crack patterns

Complex crack patterns using variational phase-field models (Gradient damage models)



Thermal shock, PRL 14



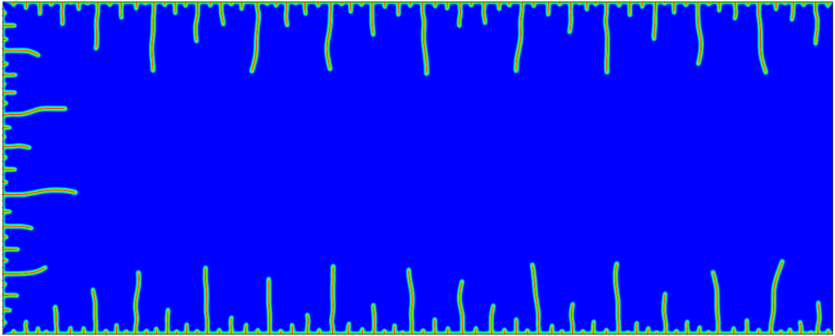
Thin film fracture and debonding, JMPS 14

Full scale simulation in 2d

Ceramic slab from Shao et al. 2011 with $\Delta T = 380\,^\circ$C

- Material : $E = 340\,\mathrm{GPa}$, $\nu = 0.22$, $G_c = 42.47\,\mathrm{Jm}^{-2}$, $\sigma_c = 342.2\,\mathrm{MPa}$, $\beta = 8 \times 10^{-6}\,\mathrm{K}^{-1}$
- Dimensions: $5\,L \times L \times 0.1\,L$, with $L = 10\,\mathrm{mm}$

$$\ell = \frac{3G_c E}{8\sigma_c^2} = 46\,\mu\mathrm{m}, \qquad \ell_0 = \frac{G_c}{E\beta^2\Delta T^2} = 14\,\mu\mathrm{m} \qquad \Rightarrow \qquad L/\ell = 215 \qquad \ell_0/\ell = 0.3$$



5 millions of elements (mesh size $\sim \ell/5$), 100 time step.

A step back: verification and validation on classical test cases

Are these models quantitively accurate?

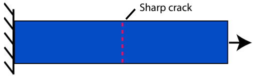
- Propagation conditions for existing cracks?
- Initiation and nucleation of new cracks?
- Scale effects?
- In linear elastic fracture mechanics, several criteria have been developed to account for experimental findings (e.g. double criterion). Should these criteria be added to variational models ?
- Are energetic criteria enough to predict crack propagation and nucleation?

Outline

- Review of gradient damage models
- Basic examples: propagation of a crack and nucleation in a traction test
- Nucleation at a V-notch
- Nucleation at a U-notch
- Effect of an elliptical hole
- Structural size effects

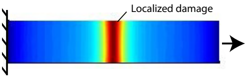
Sharp vs Smeared approaches to brittle fracture

Sharp models (Griffith)



Cracks as surfaces of sharp discontinuity of the displacement field

Smeared models (Damage)



Cracks approximated by the localisation of a smooth auxiliary field (damage).

Sharp model: Griffith

- **Global** minimisation of ($\mathcal{K}$ is the **irreversible** crack set):

  Griffith 1921, Francfort and Marigo 1998.

$$\mathcal{E}(u,\mathcal{K}) = \int_{\Omega\setminus\mathcal{K}} \frac{1}{2} A_0 \varepsilon(u)\cdot\varepsilon(u)\,dx + G_c\,\mathrm{area}(\mathcal{K})$$

Smeared models: gradient damage (phase-field)

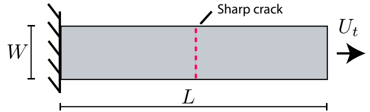
- **Local** minimisation of (α is a **irreversible** scalar damage field):

$$\{\mathcal{E}_\ell(u,\alpha) = \underbrace{\frac{1}{2}\int_\Omega (1-\alpha)^2\, A\,\varepsilon(u)\cdot\varepsilon(u)\,dx}_{\text{Strain energy}} + \underbrace{\frac{3G_c}{8}\int_\Omega \left(\frac{\alpha}{\ell} + \ell\,\nabla\alpha\cdot\nabla\alpha\right)dx}_{\text{Dissipated energy}}\}$$

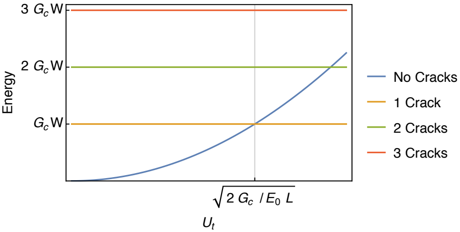
  - Mathematics (Variational regularisations, Γ-convergence):
    Mumford and Shah, 1989, Ambrosio and Tortorelli, 1990, Bourdin et al. 2000.
  - Physics: Phase-field models
    Ginzburg-Landau 1938-1950, Aranson et al., 2000; Karma et al., 2001
  - Mechanics: Damage models
    Local model, non-local models, gradient models, etc ...

Traction of a bar: Griffith model

Assume a crack set $\mathcal{K}$ in the form of n transverse cracks and a 1D bar model.



$$\mathcal{E}(u,\mathcal{K}) = \int_{\Omega\setminus\mathcal{K}} \frac{1}{2} E\, u'(x)^2\, dx + G_c W\, n(\mathcal{K})$$



Results for Griffith model

- Local minimality criterion: the bar never cracks
- Global minimality criterion: a single crack at

$$\boxed{\frac{U_G}{L} = \sqrt{\frac{2G_c}{E_0 L}}} \qquad \boxed{\sigma_G = \sqrt{\frac{2E_0\, G_c}{L}}}$$

- Global minimization is the only way to get crack nucleation without adding ad-hoc geometric features (initial test-cracks). But the maximum allowable stresses are infinite for short bar and vanishing for long bars, which is physically not acceptable (see FM98).

Gradient damage model

Total energy functional
(linearized isotropic elasticity with isotropic gradient damage)

$$\mathcal{E}_\ell(u,\alpha) = \underbrace{\frac{1}{2}\int_\Omega A(\alpha)\,\varepsilon(u)\cdot\varepsilon(u)\,dx}_{\text{Strain energy}} + \underbrace{\frac{G_c}{c_w}\int_\Omega \left(\frac{w(\alpha)}{\ell} + \ell\,\nabla\alpha\cdot\nabla\alpha\right)dx}_{\text{Dissipated energy}}, \qquad c_w = 4\int_0^1 \sqrt{w(\alpha)}\,d\alpha$$

- α, a scalar field on Ω: an internal variable representing the damage field.
- $A(\alpha) = a(\alpha)\,A_0$: the damaged elastic tensor (decreasing from $A(0) = A_0$ to $A(1) = 0$).
- $w(\alpha)$: dissipation for homogeneous damage (increasing from $w(0) = 0$).
- ℓ: internal length.

Key requirements

- stress softening: $\frac{w'(\alpha)}{s'(\alpha)}$ not increasing, $s = a^{-1}$
- finite elastic limit: $w'(0) > 0$
- finite dissipation at full damage: $w(1) < \infty$

Model retained for computations

$$a(\alpha) = (1-\alpha)^2, \qquad w(\alpha) = \cancel{\alpha^2}\ \alpha$$

$$c_w = 8/3$$

Halphen and Nguyen 1975, Fremond, Nedjar 1996; Lorentz, Andrieux 1999, Comi 2001, Nguyen and Andrieux 2005, Benallal, Marigo 2007; Pham, Marigo 2010; Lorentz, Godard 2011; Pham, Marigo 2013

Gradient damage model

Linearized isotropic elasticity with isotropic gradient damage

$$\mathcal{E}_\ell(u,\alpha) = \underbrace{\frac{1}{2}\int_\Omega \overset{(1-\alpha)^2\text{, stiffness modulation}}{a(\alpha)}\, A_0\, \varepsilon(u)\cdot\varepsilon(u)\, dx}_{\text{Elastic energy}} + \underbrace{\frac{G_c}{c_w}\int_\Omega \left(\frac{\overset{\alpha\text{, local dissipation}}{w(\alpha)}}{\ell} + \overset{\text{gradient term}}{\ell\, \nabla\alpha\cdot\nabla\alpha}\right) dx}_{\text{Dissipated energy}}$$

α, a scalar damage field, ℓ: internal length.

- Quasi-static time-discrete evolution at time t_i from the state (u_{i-1}, α_{i-1}):

$$\boxed{\min_{u\in\mathcal{U}_i,\ \alpha\geq\alpha_{i-1}} \mathcal{E}_\ell(u,\alpha), \qquad (\underline{\textbf{local}}\text{ minimization with }\textbf{unilateral constraint})}$$

- Energetic equivalence with Griffith by setting:

$$c_w = 4\int_0^1 \sqrt{w(\alpha)}\,d\alpha \overset{w(\alpha)=\alpha}{=} \frac{8}{3}$$

Halphen and Nguyen 1975, Fremond, Nedjar 1996; Lorentz, Andrieux 1999, Comi 2001, Nguyen and Andrieux 2005, Benallal, Marigo 2007; Pham, Marigo 2010; Lorentz, Godard 2011; Pham, Marigo 2013

Minimization with bound constraints: variational inequalities

1 degree of freedom system

Example: Scalar function of a scalar variable
$f : x \in \mathcal{R} \rightarrow f(x) \in \mathcal{R}$

$$\boxed{x^* = \underset{x \geq \bar{x}}{\operatorname{argmin}} f(x)}$$

First order optimality conditions:

- Minimality implies non-negative variations:

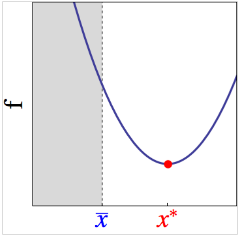
$$f(x) - f(x^*) \simeq \boxed{f'(x^*)(x - x^*) \geq 0, \qquad \forall x \geq \bar{x}}$$

- Equivalent KKT conditions:

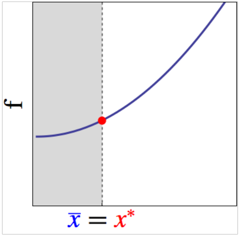
$$\boxed{f'(x^*) \geq 0 \quad (x^* - \bar{x}) \geq 0 \quad f'(x^*)(x^* - \bar{x}) = 0}$$

This is a non-linear problem. If f is convex the solution is unique.

Case A: $x^* > \bar{x} \Rightarrow f'(x^*) = 0$



Case B: $x^* = \bar{x} \Rightarrow f'(x^*) \geq 0$



Gradient damage model: evolution problem

First order optimality conditions

Equilibrium equations (u-variation)

$$\mathrm{div}\sigma = 0 \text{ in } \Omega, \qquad \sigma n = f \quad \text{on} \quad \partial_f\Omega, \quad \text{with} \quad \sigma = a(\alpha)A_0\varepsilon(u) \tag{1}$$

Damage criterion and Kuhn-Tucker conditions (α-variation)

$$\text{In } \Omega \quad : \quad \alpha - \alpha_{i-1} \geq 0, \quad \mathrm{D} \geq 0, \quad (\alpha - \alpha_{i-1})\,\mathrm{D} = 0, \tag{2}$$

$$\text{On } \partial\Omega \quad : \quad \alpha - \alpha_{i-1} \geq 0, \quad \frac{\partial\alpha}{\partial n} \geq 0, \quad \frac{\partial\alpha}{\partial n}(\alpha - \alpha_{i-1}) = 0, \tag{3}$$

where $\quad \mathrm{D}(\varepsilon, \alpha, \Delta\alpha) = \dfrac{a'(\alpha)}{2}A_0\varepsilon\cdot\varepsilon + \dfrac{G_c}{c_w}\left(\dfrac{w'(\alpha)}{\ell} - 2\ell\Delta\alpha\right)$

The energetic criterion (local energy minimality conditions) implies:

- **Stress domain for homogenous damage**:

$$\mathrm{D}(\varepsilon, \alpha, 0) \geq 0 \quad \Rightarrow \quad A_0^{-1}\sigma\cdot\sigma \leq -\frac{2\ G_c w'(\alpha)}{c_w\,\ell\,(a^{-1})'(\alpha)}$$

- **Elastic limit** in unixial traction:

$$\sigma_c = \sqrt{\frac{2\,G_c E\,w'(0)}{\ell\,c_w\,(a^{-1})'(0)}} \Rightarrow \boxed{\sigma_c = \sqrt{\frac{3G_c E}{8\ell}}}$$

- Stability (second order condition) depends on the gradient term (and ℓ)

Gradient damage model: evolution problem

First order optimality conditions

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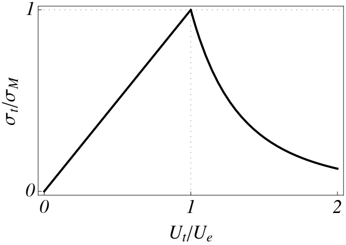
Considered constitutive models

Homogeneous response in 1d traction

AT1 - model

$$w(\alpha) = \alpha, \quad a(\alpha) = (1-\alpha)^2$$



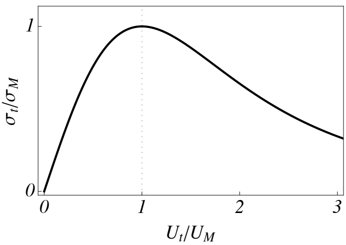
- Finite elastic limit

$$\sigma_c = \sigma_M = \sqrt{\frac{3 G_c E_0}{8\,\ell}}$$

- Linear elastic followed by softening

AT2 - model

$$w(\alpha) = \alpha^2, \quad a(\alpha) = (1-\alpha)^2$$

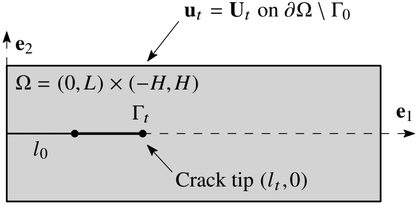


- Null elastic limit
- Hardening followed by softening
- Used in most of the papers on phase-field fracture

Pham, Marigo, Maurini 2011; Lorentz, Godard 2011

Elementary verification tests

Propagation of an existing crack



Nucleation in a homogenous bar

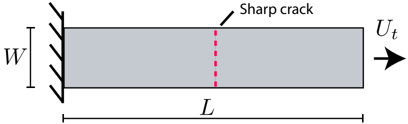
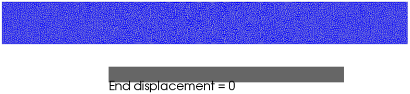
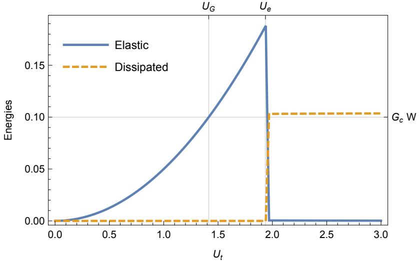


Illustration: traction of a bar



- $L = 1, W = 0.1, \ell = 0.05$
- Element size 0.005
- Critical load:

$$\boxed{\frac{U_c}{L} = \sqrt{\frac{3G_c}{8E_0\,\ell}}} \qquad \boxed{\sigma_c = \sqrt{\frac{3G_c}{8E_0\,\ell}}}$$

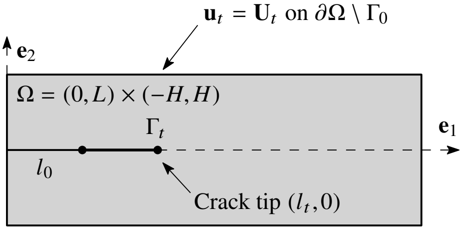


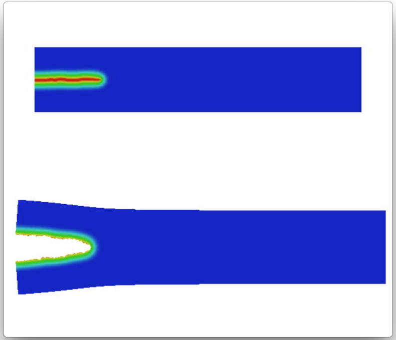
- **Elastic phase** (homogeneous damage) $\Rightarrow$ **Loss of stability** $\Rightarrow$ **Localized solution** (fracture)
- The dissipated energy in the localized solution is equal to the crack length ($G_c = 1$)
- Crack nucleation is a structural stability problem

Propagation of a straight crack

Surfing experience

- Consider a slab with an initial crack l_0
- Impose asymptotic mode-I displacement on the boundary focussed on a crack tip moving at a constant speed v



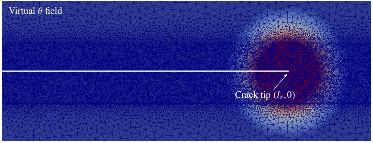


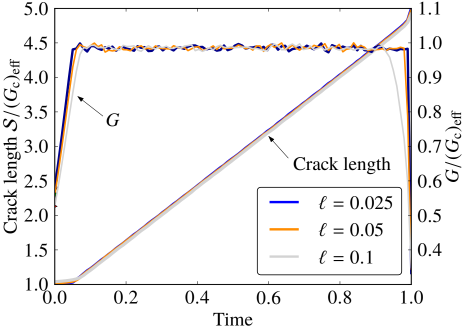
Top: damage field. Bottom: apply displacement and remove element with $\alpha > 0.9$

Propagation of a straight crack

Evaluate the Energy Release Rate (ERR) through G-θ integral (Destuynder et al., 1983), where θ is an auxiliary field defining a virtual displacement of the domain with

$$\theta = \begin{cases} \underline{e}_1 & \text{close to the tip (red region)} \\ \underline{0} & \text{far from the tip (blue region)} \end{cases}$$

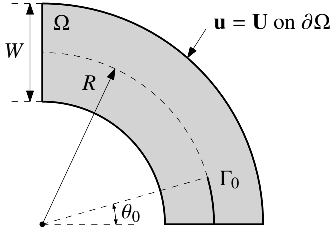




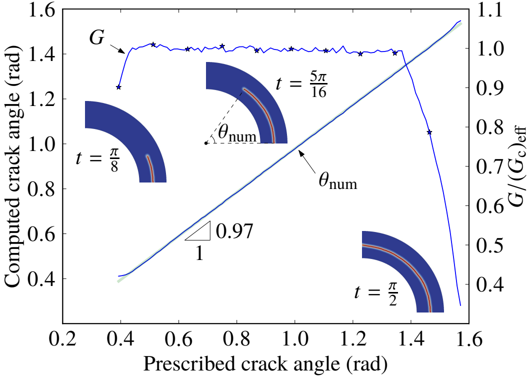
$$G = \int_\Omega \left(\frac{a(\alpha)}{2} A_0 \varepsilon(u) \cdot \varepsilon(u) \mathrm{div}\theta - a(\alpha) A_0 \varepsilon(u) \cdot (\nabla u \nabla \theta) \right) dx$$

Griffith and gradient damage models give the same evolution:

$\boxed{G = G_c}$, no dependence on ℓ



(a)

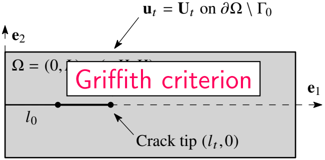


(b)

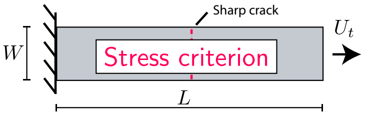
Loading: asymptotic mode-I displacement for propagation along a circular path

Initiation and nucleation tests

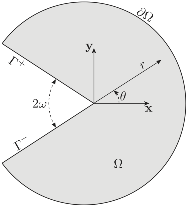
Propagation of an existing crack



Nucleation in a homogenous bar

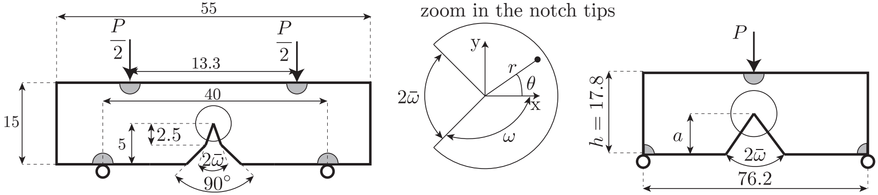


Nucleation at a V-notch ?



Nucleation at a notch

3- and 4-point bending tests

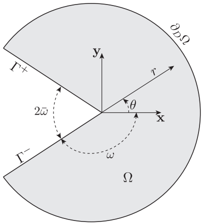


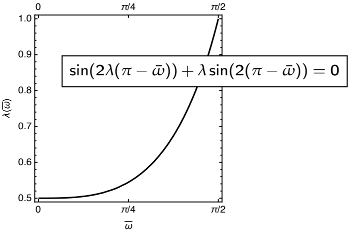
Experimental results from:

- 4-point bending on Duraluminium by Yosibash et al, IJF 2004
- 3-point bending on PMMA by Dunn at al IJSS 1997 and IJF 1997

Nucleation at a notch

Pac-man geometry for the study of the crack nucleation at a notch





Asymptotic solution in linear elasticity

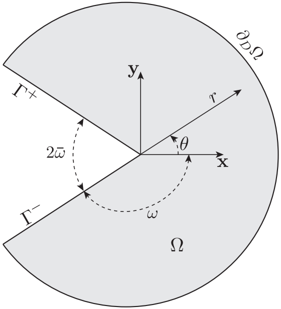
$$\sigma_{\theta\theta}=kr^{\lambda-1}F(\theta),\quad \sigma_{rr}=kr^{\lambda-1}\frac{F''(\theta)+(\lambda+1)F(\theta)}{\lambda(\lambda+1)},\quad \sigma_{r\theta}=-kr^{\lambda-1}\frac{F'(\theta)}{(\lambda+1)},$$

where $\boxed{k=\left.\dfrac{\sigma_{\theta\theta}}{(2\pi\, r)^{\lambda-1}}\right|_{\theta=0}}$ is a generalized stress intensity factor

$$F(\theta)=(2\pi)^{\lambda-1}\frac{\cos((1+\lambda)\theta)-f(\lambda,\bar{\omega})\cos((1-\lambda)\theta)}{1-f(\lambda,\bar{\omega})},\quad f(\lambda,\bar{\omega})=\frac{(1+\lambda)\sin((1+\lambda)(\pi-\bar{\omega}))}{(1-\lambda)\sin((1-\lambda)(\pi-\bar{\omega}))}.$$

D. Leguillon and E. Sanchez-Palencia, 1987

Nucleation at a notch



Computational method

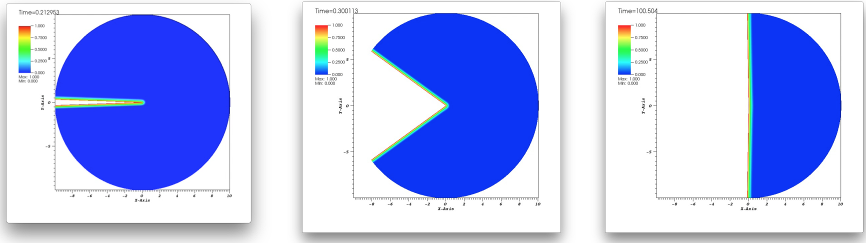
- Assume separation of scale between inner damage problem and outer linear elastic problem
- Apply asymptotic linear elastic solution at the boundary
- Generalized SIF k is the loading parameter (time)
- Ω large enough, mesh small enough

- The stress are singular for $\bar{\omega} < \pi/2$
- For $\bar{\omega} = 0$ (a crack), ERR > 0: a crack propagates according to Griffith model.
- For any $\bar{\omega} > 0$, ERR$=0$: the stresses are not singular enough to release enough elastic energy for a "Griffith" crack.
- For $\bar{\omega} \simeq \pi/2$ the stress field is almost uniaxial. The critical stress value at nucleation can be estimated by the one of a bar in traction:

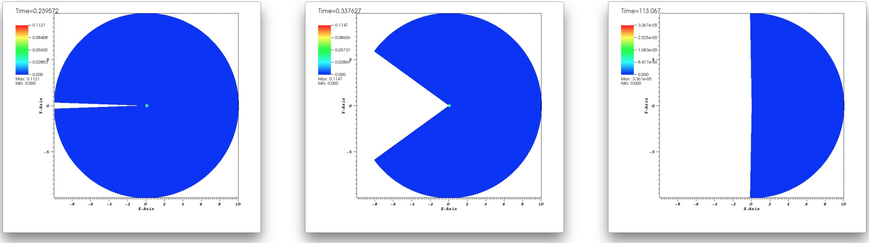
$$\sigma_c = \sqrt{\frac{3EG_c}{8\ell}}$$

Nucleation at a notch

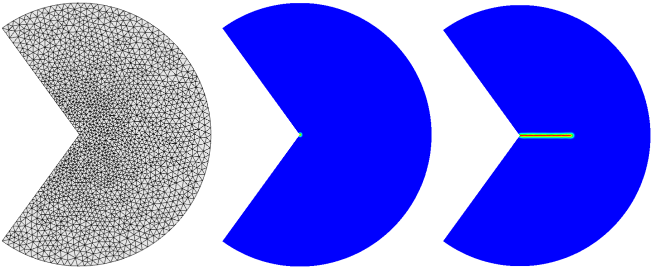
Damaged crack lips: $\alpha = 1$ on Γ

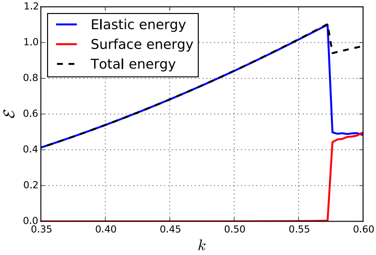


Free crack lips: $\dfrac{\partial \alpha}{\partial n} = 0$ on Γ



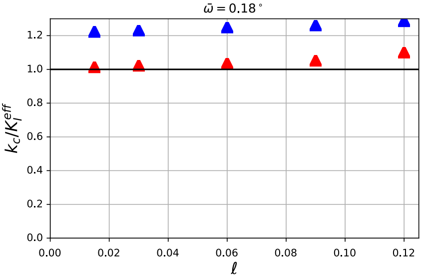
Critical loading at nucleation

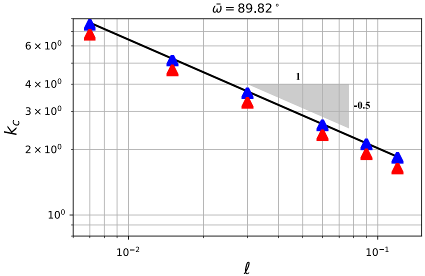




Nucleation at a notch: critical loading at nucleation

Recovering the limit cases : $\bar{\omega} \to 0$ (crack) and $\bar{\omega} \to \pi/2$ (bar)





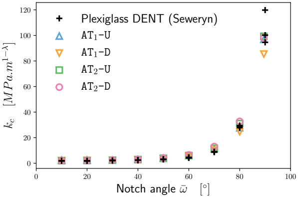
Crack: $G = G_c$

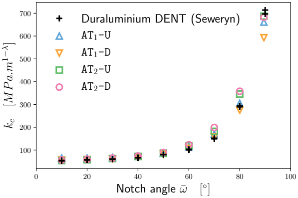
Bar: $\sigma = \sigma_c \propto \sqrt{\dfrac{G_c E}{\ell}}$

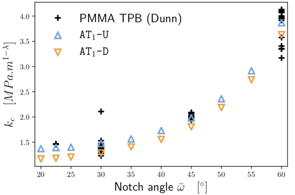
AT1 model, Red : damaged crack lips, blue : undamaged crack lips

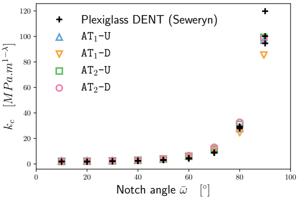
Comparison with experimental results: V-notch

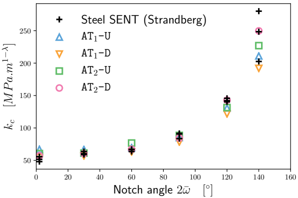
Critical generalised stress intensity factor at nucleation

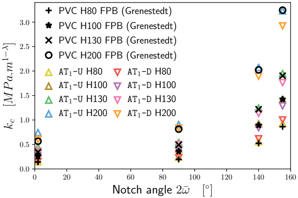






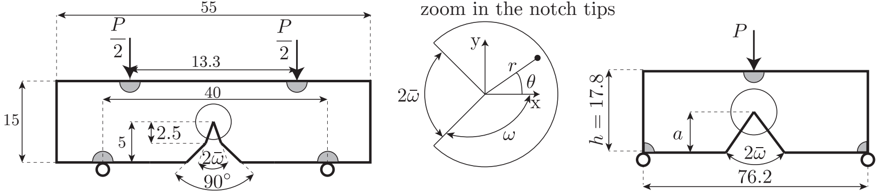


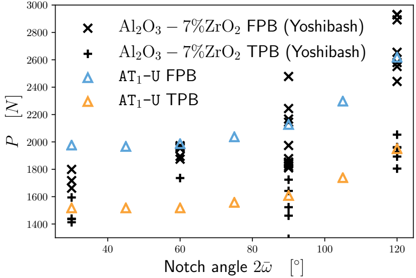


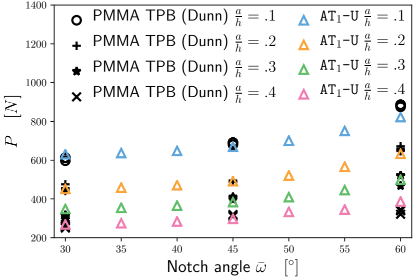


Full structure numerical computation

Critical force P at initiation

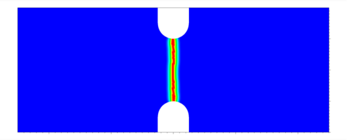


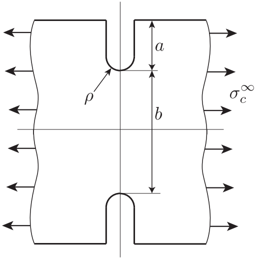


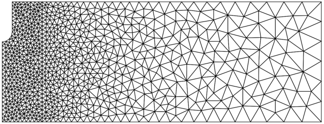


	E [GPa]	ν	K_I [MPa$\sqrt{\text{m}}$]	σ_c [MPa]	ℓ (AT1 model)[μm]
PMMA	2.3	0.36	1.028	124	26
Duraluminium	350	0.236	4.1	290	75

U-notch: DENT test



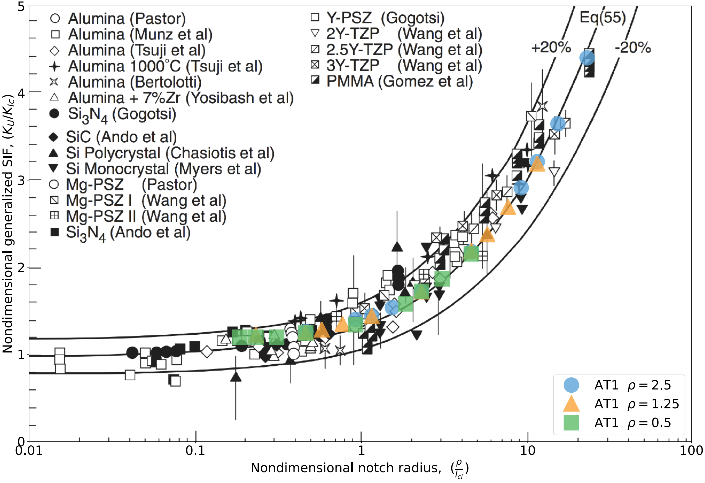




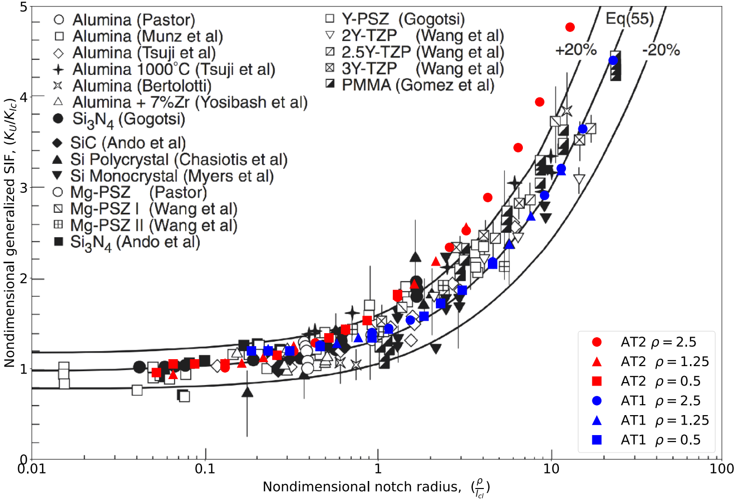
- Consider the regime $a \gg \ell$, $a \gg \rho$
- Study the influence of ρ/ℓ
- Simplify the problem by using asymptotic solution in linear elasticity as a BC

U-notch

Gradient damage vs experimental results for AT1



U-notch



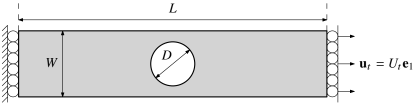
Alumina (Pastor)
Alumina (Munz et al)
Alumina (Tsuji et al)
Alumina 1000°C (Tsuji et al)
Alumina (Bertolotti)
Alumina + 7%Zr (Yosibash et al)
Si3N4 (Gogotsi)
SiC (Ando et al)
Si Polycrystal (Chasiotis et al)
Si Monocrystal (Myers et al)
Mg-PSZ (Pastor)
Mg-PSZ I (Wang et al)
Mg-PSZ II (Wang et al)
Si3N4 (Ando et al)
Y-PSZ (Gogotsi)
2Y-TZP (Wang et al)
2.5Y-TZP (Wang et al)
3Y-TZP (Wang et al)
PMMA (Gomez et al)
Eq(55)
+20%
-20%
AT2 ρ = 2.5
AT2 ρ = 1.25
AT2 ρ = 0.5
AT1 ρ = 2.5
AT1 ρ = 1.25
AT1 ρ = 0.5
Nondimensional generalized SIF, (KU/KIc)
Nondimensional notch radius, (ρ/lcl)
0
1
2
3
4
5
0.01
0.1
1
10
100

A first summary

Some conclusions from U- and V- notches

1. The local energy minimisation principle on the gradient-damage model conciliates the stress and toughness criteria.
2. The results are in quantitative agreement with experiments, on many materials and geometries.
3. No need for ad-hoc nucleation criteria in this framework.

Influence of imperfections: traction of bar with an hole

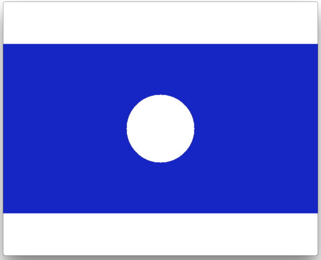


$\sigma_{\max} \simeq 3\sigma_\infty$ for $D \ll W$

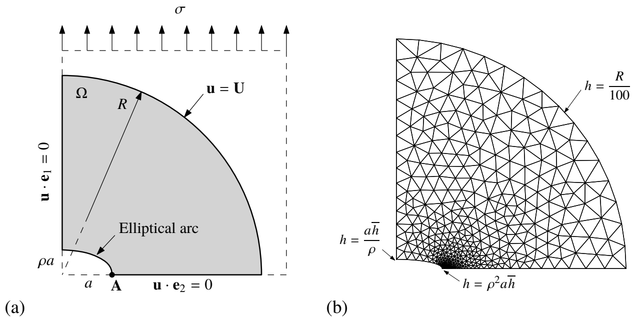
- Critical loading of a bar without the hole:

$$U_0(\ell) = L\sqrt{\frac{3G_c}{E8\ell}}, \qquad \sigma_0(\ell) = \sqrt{\frac{3G_cE}{8\ell}}$$

- Two key parameters: $\dfrac{D}{W}$, $\dfrac{\ell}{D}$



Crack nucleation in an infinite domain containing an elliptical hole



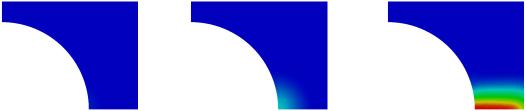
(a) Problem setting and loading conditions. (b) Typical mesh used for numerical experiment

- An analytical solution is available, with maximum stress at A given by

$$\boxed{\sigma_{\theta\theta} = \sigma\left(1 + \frac{2}{\rho}\right)}$$

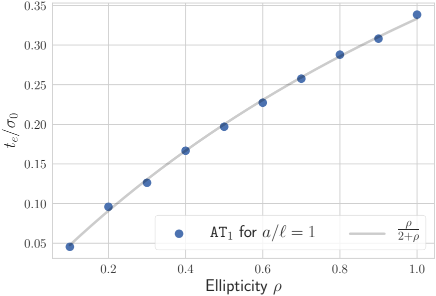
- We apply the asymptotic solution for linear elasticity on the boundary

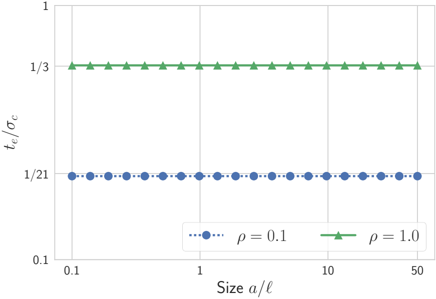
Crack nucleation in an infinite domain containing an elliptical hole



Elastic phase damage nucleating crack nucleating

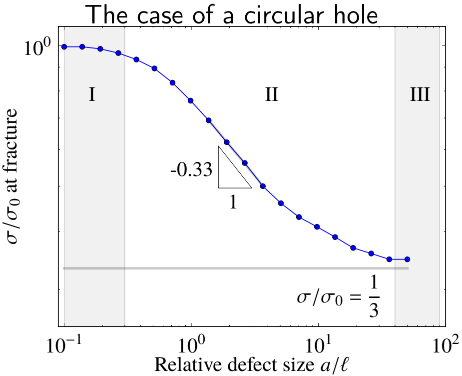
Critical load for damage nucleation





Crack nucleation in an infinite domain containing an elliptical hole

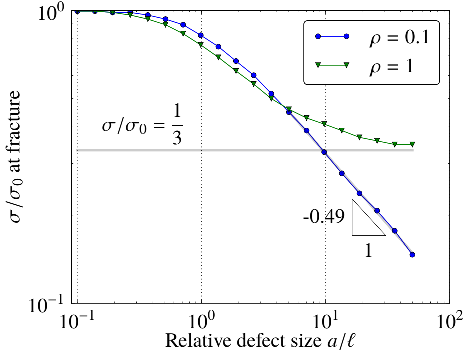
Critical load for the nucleation of a full crack with $\alpha = 1$ on a band



- I (small hole) - $\sigma = \sigma_0$: The effect of the hole is filtered out in the relative large processing zone. Nucleation as in a homogeneous bar.
- II ($a \sim \ell$) - Non-trivial transition zone with the material scale effect
- III (large hole) - $\sigma = \sigma_0/3$: Nucleation at end of the elastic phase.

Crack nucleation in an infinite domain containing an elliptical hole

Critical load for the crack nucleation: shape effect

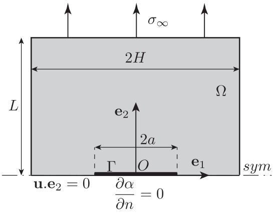


- For $\rho = 0.1$ and $a \gg \ell$ we recover the scaling law of a crack: $\boxed{\sigma \propto \sqrt{\frac{EG_c}{a}}}$

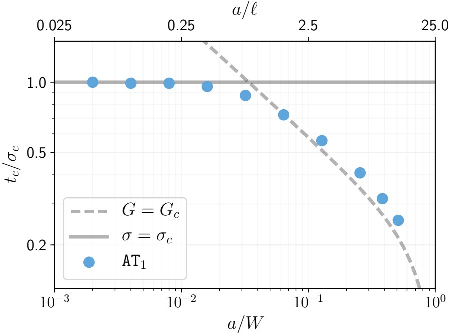
Crack in a domain of finite width and scale effects

Critical load for crack initiation

Results for $H = 1$, $\ell = 0.04$



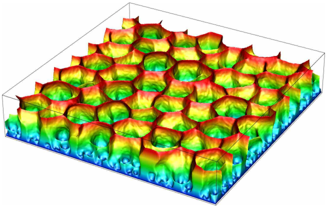
$$\sigma_\infty^G = \sqrt{\frac{\bar{E}\, G_c \cos\left(\frac{a\pi}{2H}\right)}{a\pi}}$$

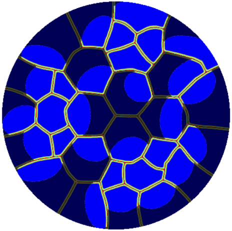


- $a \ll \ell$ Stress criterion (no effect of the defect)
- $a \gg \ell$ Griffith criterion (no effect of the the internal length)
- $a \simeq \ell$ "Mixed" regime

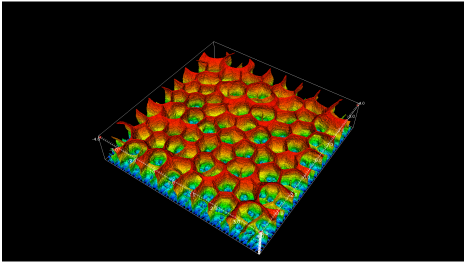
Conclusions

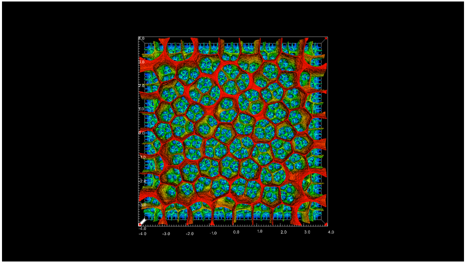
- Quantitively accurate results for crack nucleation on different geometries.
- V-notch and U-notch experimental results can be used to accurately estimate the parameters of the models.
- No need for additional local ad-hoc nucleation criterion, the energy minimisation principle implies both.
- This is a nonlinear damage model, not only a criterion for the limit of validity of linear elasticity: can predict post-critical behaviour.
- Crack nucleation is a structural stability problem.





Movies





End

- FEniCS/python based, parallel open-source demo codes in the form of interactive on-linejupyter-notebook available here (no installation required) https://notebooks.azure.com/cmaurini/libraries/varfrac
- Scripts reproducing most of the results of this presentations are available (thanks to Tianyi Li and Erwan Tanné): `https://bitbucket.org/cmaurini/gradient-damage`
- See also Blaise Bourdin's fortran90 code (`https://bitbucket.org/bourdin/mef90-sieve`)
- Tanné, E., Li, T., Bourdin, B., Marigo, J.-J., Maurini, C. (2018). Crack nucleation in variational phase-field models of brittle fracture. Journal of the Mechanics and Physics of Solids, 110, 80–99. https://doi.org/10.1016/j.jmps.2017.09.006