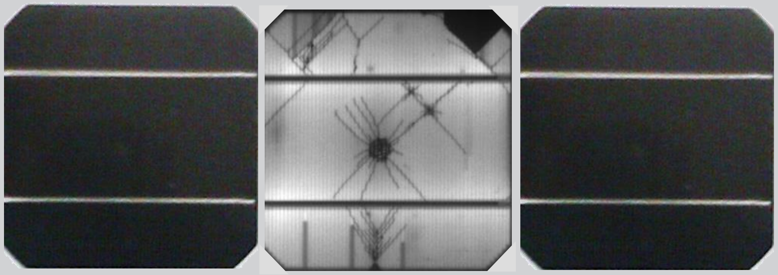
Phase field approach to brittle fracture and cohesive zone models for fracture mechanics in heterogeneous materials and composites



Marco Paggi

IMT School for Advanced Studies Lucca

University of Portsmouth, UK

January 17, 2018

SCUOLA ALTI STUDI LUCCA

IMT (Institutions, Markets, Technologies) in a nutshell

SCUOLA NORMALE SUPERIORE

IMT SCUOLA ALTI STUDI LUCCA

Sant'Anna Scuola Universitaria Superiore Pisa

GSSI

IUSS Sapere Aude Istituto Universitario di Studi Superiori Pavia

SISSA

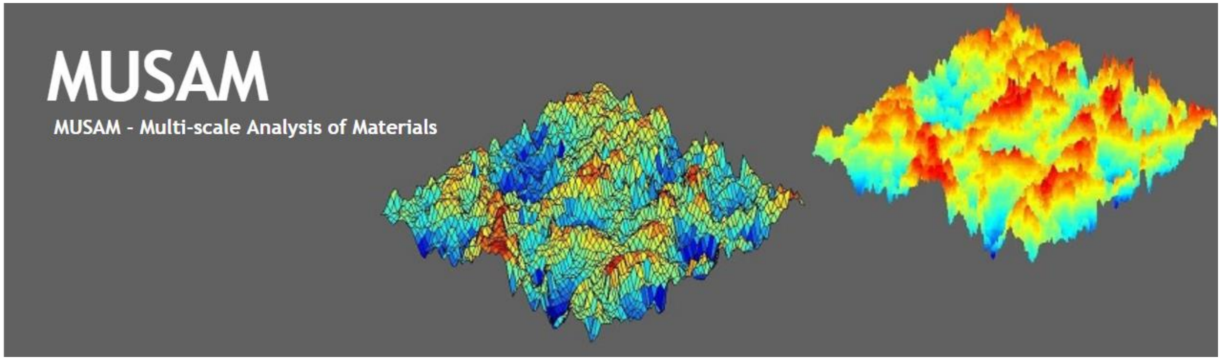
One of the 6 Italian public schools for advanced studies:

- 15 permanent faculty members + 3 tenure-track assistant professors
- 36 PhD students per year
- One interdisciplinary PhD programme in Systems Science (mechanics, optimization and control, computer science)

IMT (Institutions, Markets, Technologies) in a nutshell

7 Research units:

DYSCO, MUSAM, SYSMA, AXES, LYNX, NETWORKS, MOMILAB



Multi-scale Analysis of Materials
MUSAM Research unit

- **M. Paggi**, Full Professor
- **A. Bacigalupo**, Assistant Professor

Post-docs

- **C. Borri**
- **M. Gagliardi**
- **F. Biancalani**

PhD students

- **V. Carollo**
- **P. Cinat**
- **V. Govindarajan**
- **R. Del Toro**
- **N. Dardano**
- **T. Guillen Hernandez**
- **M. Marulli**
- **J. Bonari**

Former staff

- **P. Budarapu** (tenure-track assistant prof., Indian Institute of Technology, Bhubaneswar)
- **O.S. Ojo** (post-doc, University of Limerick, Ireland)
- **L. Morini** (post-doc, University of Cardiff, UK)
- **P. Lenarda** (post-doc, IIT Genova)
- **F. Fantoni** (post-doc, University of Brescia)
- **I. Berardone** (post-doc, University of Bologna)

IMT SCUOLA ALTI STUDI LUCCA

MUSAM-Lab

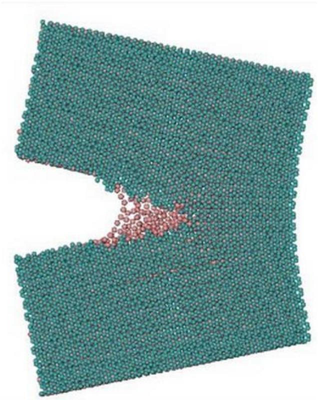
http://www.imtlucca.it/research/laboratories/musam-lab

European Research Council
Established by the European Commission
Supporting top researchers from anywhere in the world

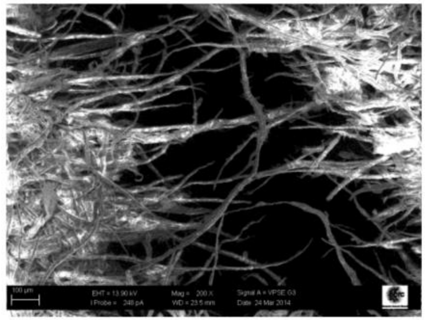
- **3D confocal-interferometric profilometer (LEICA, DCM 3D)**
- **Scanning Electron Microscope (ZEISS, EVO MA15)**
- **Micromechanical testing stage (DEBEN, 5000S)**
- **Universal testing machine with a thermostatic chamber (Zwick/Roell, Z010TH) and a peeling test setup**
- **Thermocamera (FLIR, T640bx)**
- **Photocamera for electroluminesce (PCO, 1300 Solar)**
- **3D displacement correlation technique (Correlated Solutions, VIC3D)**

IMT SCUOLA ALTI STUDI LUCCA

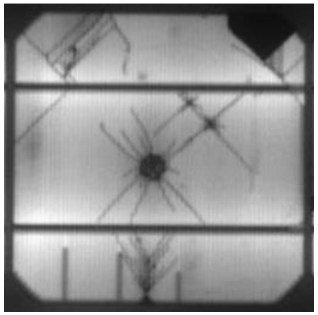
Research topics



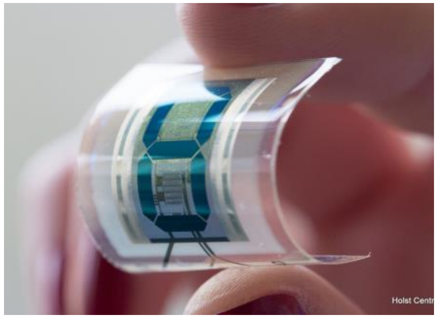
Graphene and thermal-barrier coatings



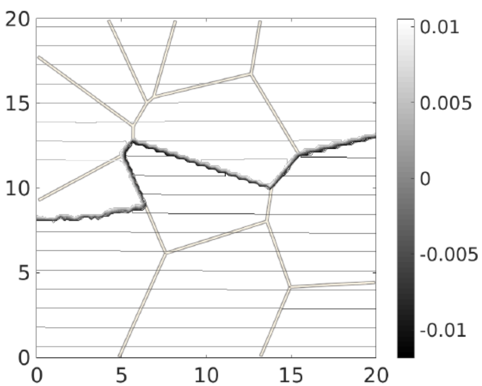
Fibrous materials (paper tissue)



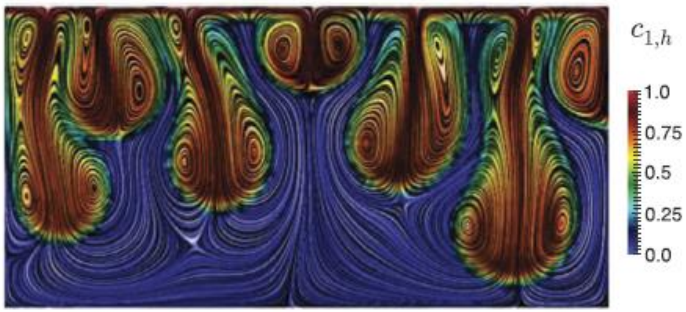
Durability of photovoltaics



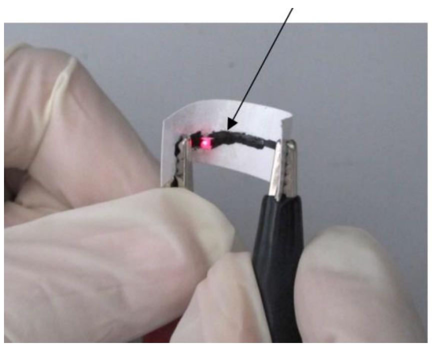
Flexible electronics



Fracture of polycrystals

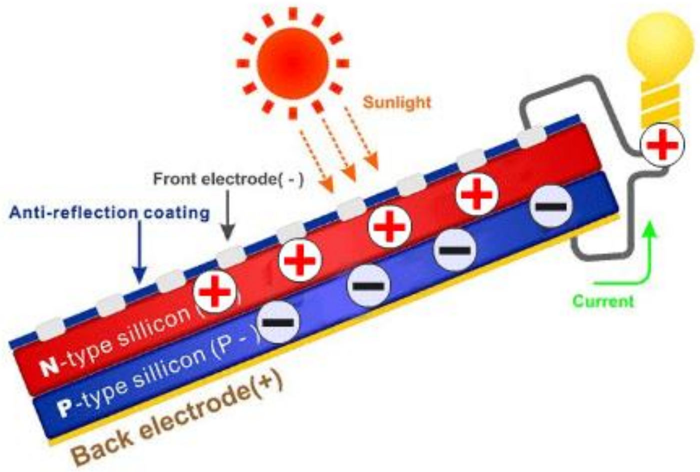


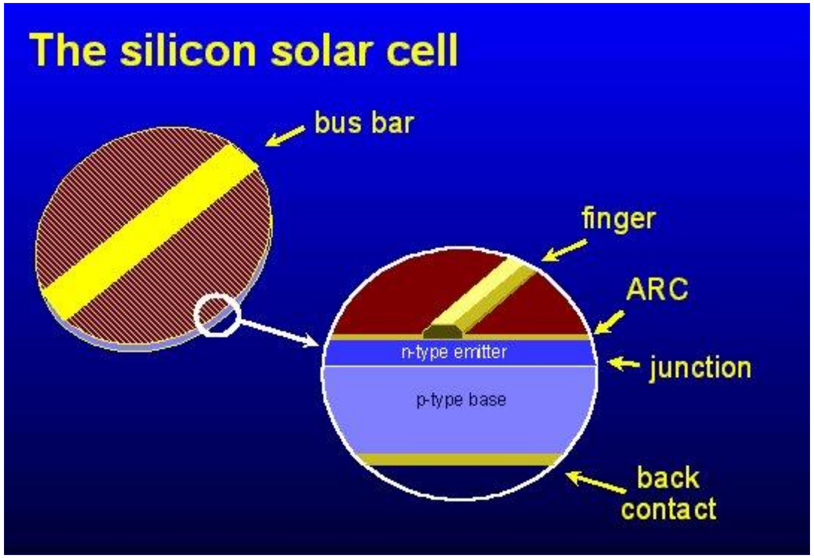
Reaction-diffusion systems (for fluids and solids)

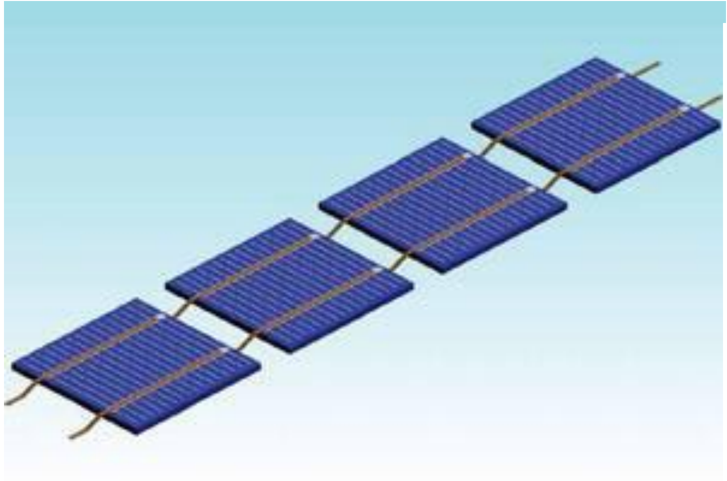


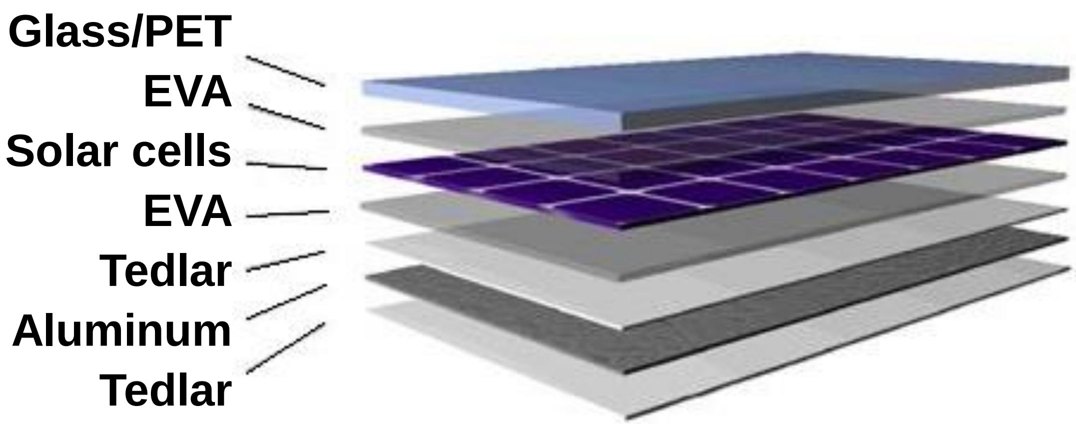
Graphene-based printable electronics

Photovoltaics (PV)

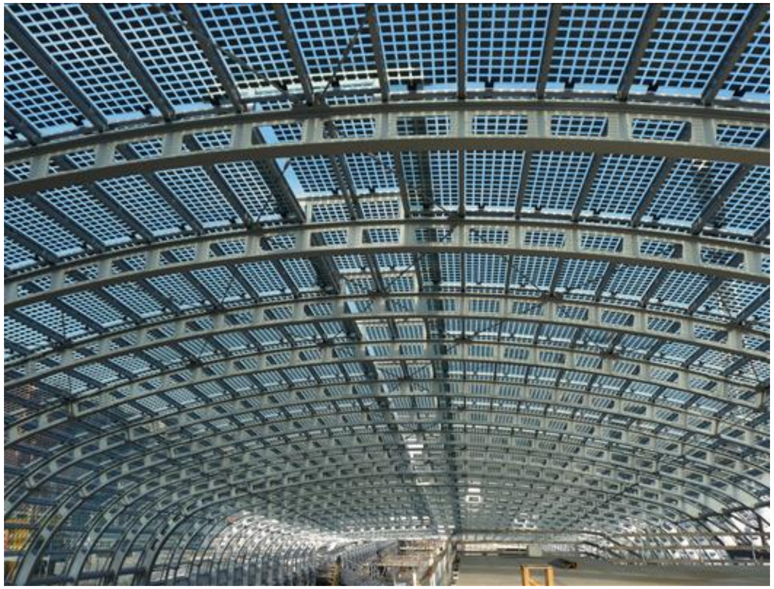








Applications:
from PV parks to building integrated PV



Endorsement and collaborations

International Energy Agency
Photovoltaic Power Systems Programme (PVPS)
Task 13 on Performance and Reliability of Photovoltaic Systems

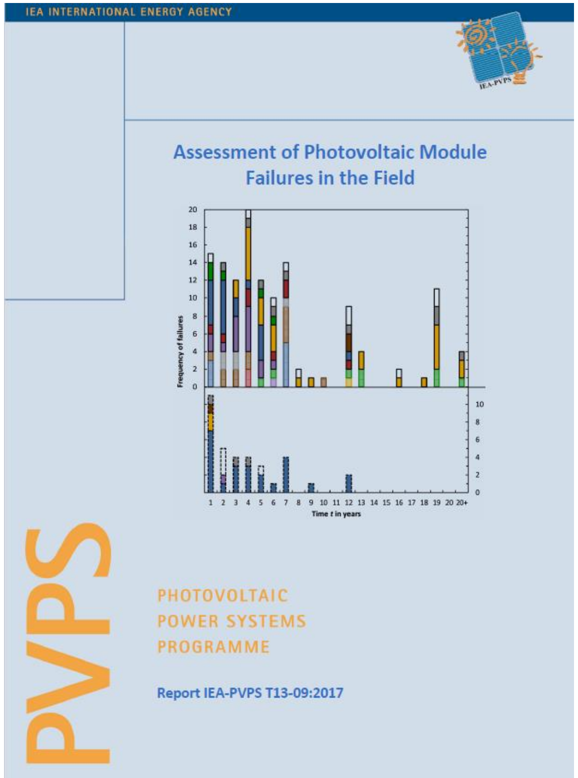
Joint Research Centre
Institute for Energy and Transport

Institute for Solar Energy Research
Hamelin, Germany

Solbian Energie Alternative S.r.l.
Avigliana, Italy

Applied Materials Italia S.r.l.
Olmi di S. Biagio di Callalta, Italy

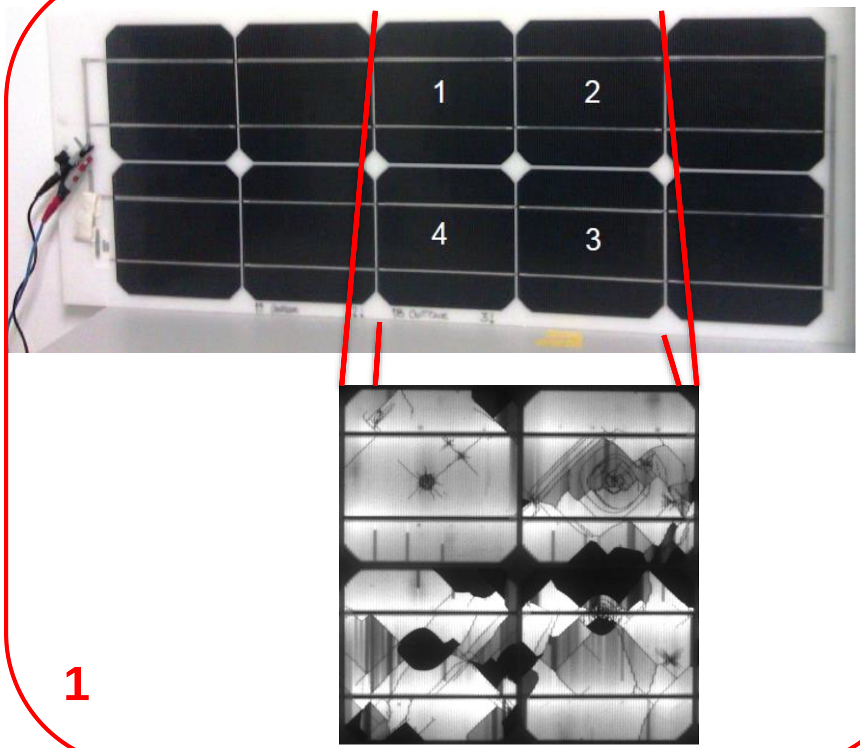
Jabil, Industrial and Energy
San Petersburg, Florida, USA



Durability

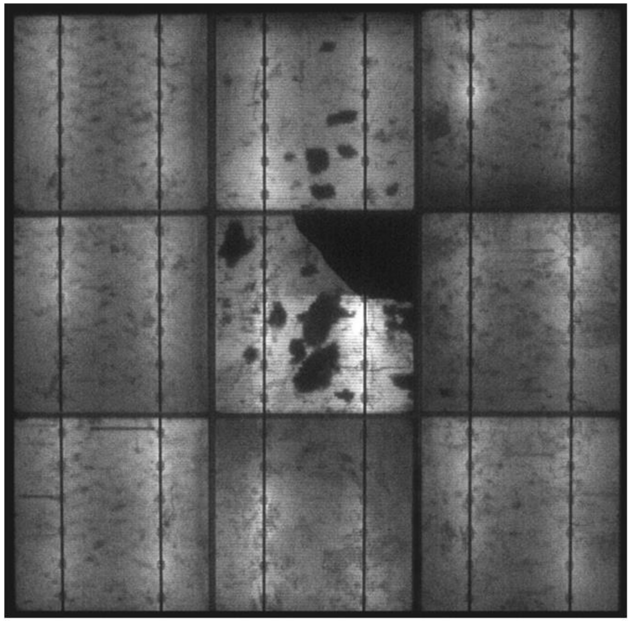
Some failure modes of PV modules:

1. Cracks
2. Decohesion of the encapsulant
3. Moisture-induced degradation



1

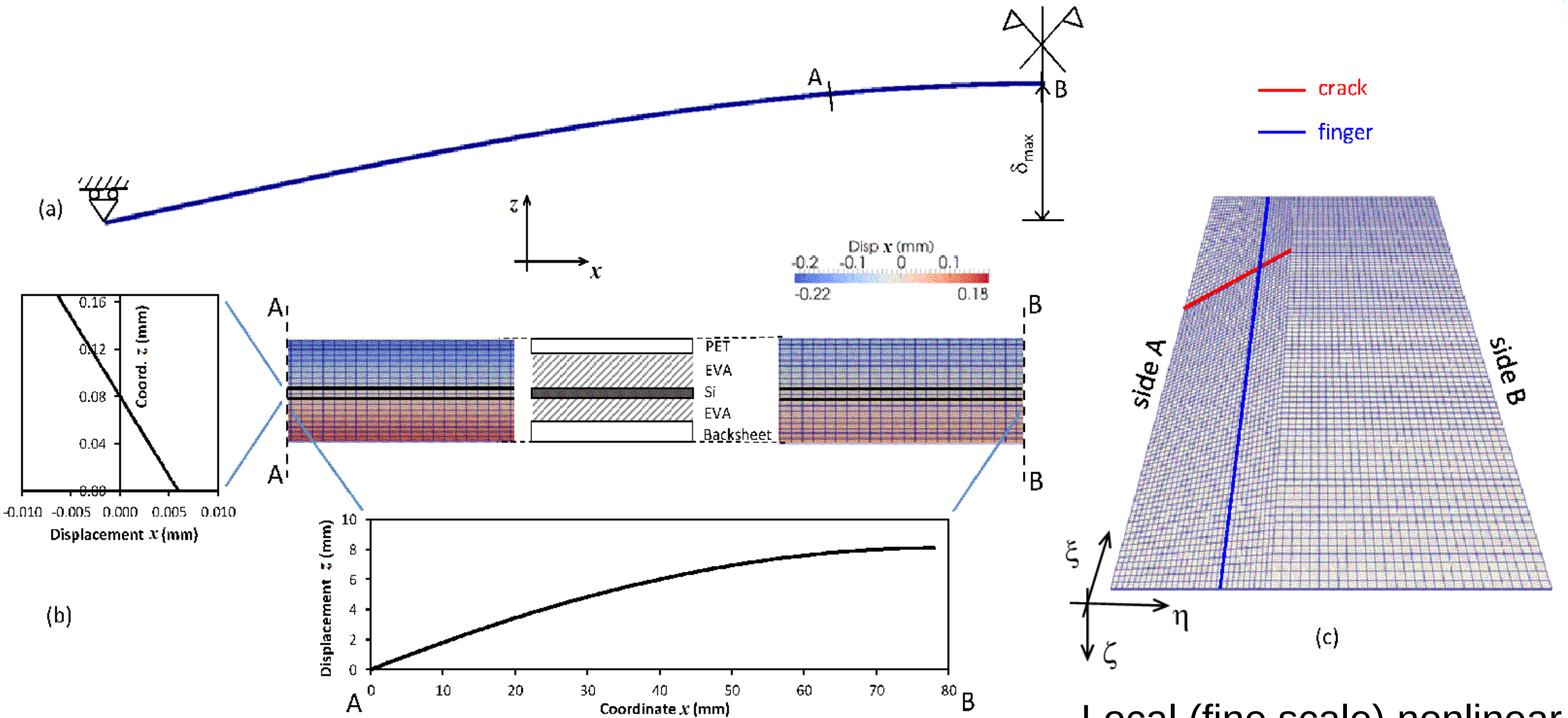
2



3

Computational methods for stress analysis and fracture mechanics of shells

Global/local finite element approach

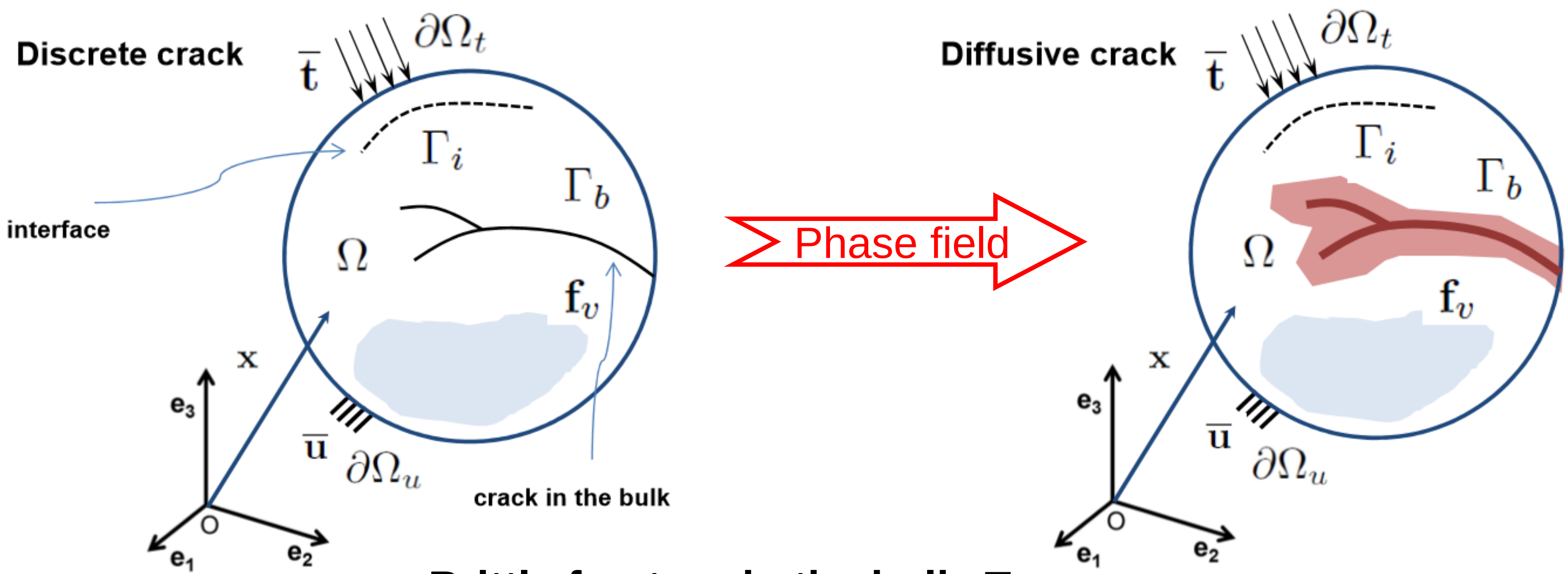


Global (coarse scale) FE model

Local (fine scale) nonlinear FE model of each solar cells

Paggi M, Berardone I, Corrado M (2016) A global/local approach for the prediction of the electric response of cracked solar cells in photovoltaic modules under the action of mechanical loads. Eng. Fract. Mech., 168:40-57.

Fracture of polycrystalline solar cells: a variational approach



- **Brittle fracture in the bulk, Γ_b**
- **Cohesive fracture along pre-existing interfaces, Γ_i**

B. Bourdin, G.A. Francfort, J.J. Marigo (2008) J. Elast. 91:5

C. Miehe, M. Hofacker, F. Welschinger (2010) CMAME 199:2765

M. Paggi, J. Reinoso (2017) Revisiting the problem of a crack impinging on an interface: a framework for the interaction between the phase field approach for brittle fracture and the interface cohesive zone model, CMAME, 321:145

Fracture of polycrystalline solar cells: a variational approach

$$\Pi(\mathbf{u},\Gamma) = \Pi_\Omega(\mathbf{u},\Gamma) + \Pi_\Gamma(\Gamma) = \int_{\Omega\backslash\Gamma} \psi^e(\boldsymbol{\varepsilon})\,\mathrm{d}\Omega + \int_\Gamma \mathcal{G}_c\,\mathrm{d}\Gamma$$

Elastic strain energy density

Dissipated energy due to fracture

$$\Pi_\Gamma = \Pi_{\Gamma_b} + \Pi_{\Gamma_i} = \int_{\Gamma_b} \mathcal{G}_c^b(\mathbf{u},\mathfrak{d})\,\mathrm{d}\Gamma + \int_{\Gamma_i} \mathcal{G}^i(\mathbf{g},\mathfrak{d})\,\mathrm{d}\Gamma$$

Dissipated energy in the bulk (Griffith fracture)

Dissipated energy along interfaces (CZM)

Contribution to the functional related to the bulk:

$$\Pi_b(\mathbf{u},\Gamma_b) = \Pi_\Omega(\mathbf{u},\Gamma_b) + \Pi_{\Gamma_b}(\Gamma_b) = \int_{\Omega\backslash\Gamma} \psi^e(\boldsymbol{\varepsilon})\,\mathrm{d}\Omega + \int_{\Gamma_b} \mathcal{G}_c^b(\mathbf{u},\mathfrak{d})\,\mathrm{d}\Gamma$$

SCUOLA ALTI STUDI LUCCA

(1) phase field for brittle fracture in the bulk

$$\Pi_b(\mathbf{u},\Gamma_b) = \Pi_\Omega(\mathbf{u},\Gamma_b) + \Pi_{\Gamma_b}(\Gamma_b) = \int_{\Omega\backslash\Gamma} \psi^e(\boldsymbol{\varepsilon})\,\mathrm{d}\Omega + \int_{\Gamma_b} \mathcal{G}_c^b(\mathbf{u},\mathfrak{d})\,\mathrm{d}\Gamma$$

Phase field (nonlocal) regularization of energy dissipation in the bulk:

$$\Pi_b(\mathbf{u},\mathfrak{d}) = \int_\Omega \psi(\boldsymbol{\varepsilon},\mathfrak{d})\,\mathrm{d}\Omega + \int_\Omega \mathcal{G}_c^b \gamma(\mathfrak{d},\nabla_\mathbf{x}\mathfrak{d})\,\mathrm{d}\Omega$$

$$\gamma(\mathfrak{d},\nabla_\mathbf{x}\mathfrak{d}) = \frac{1}{2l}\mathfrak{d}^2 + \frac{l}{2}\|\nabla_\mathbf{x}\mathfrak{d}|^2$$ **Crack density functional**

(1) phase field for brittle fracture in the bulk

Positive-negative decomposition of the strain energy (Miehe, 2010):

$$\psi(\boldsymbol{\varepsilon}, \mathfrak{d}) = \mathfrak{g}(\mathfrak{d})\psi_+^e(\boldsymbol{\varepsilon}) + \psi_-^e(\boldsymbol{\varepsilon})$$

$$\psi_+^e(\boldsymbol{\varepsilon}) = \frac{\lambda}{2}\left(\langle \mathrm{tr}[\boldsymbol{\varepsilon}]\rangle_+\right)^2 + \mu \mathrm{tr}[\boldsymbol{\varepsilon}_+^2]$$

$$\psi_-^e(\boldsymbol{\varepsilon}) = \frac{\lambda}{2}\left(\langle \mathrm{tr}[\boldsymbol{\varepsilon}]\rangle_-\right)^2 + \mu \mathrm{tr}[\boldsymbol{\varepsilon}_-^2]$$

Degradation function (Miehe, 2010): $\mathfrak{g}(\mathfrak{d}) = (1-\mathfrak{d})^2 + \mathcal{K}$

Stress tensor:

$$\boldsymbol{\sigma} := \frac{\partial \hat{\psi}}{\partial \boldsymbol{\varepsilon}} = \mathfrak{g}(\mathfrak{d})\boldsymbol{\sigma}_+ + \boldsymbol{\sigma}_- \qquad \boldsymbol{\sigma}_\pm = \lambda\left(\langle \mathrm{tr}[\boldsymbol{\varepsilon}]\rangle_\pm\right)\mathbf{1} + 2\mu\boldsymbol{\varepsilon}_\pm$$

(2) Cohesive Zone Model for interfaces

$$\boxed{\sigma = \begin{cases} k_n \dfrac{g_n}{g_{nc}}, & \text{if } 0 < \dfrac{g_n}{g_{nc}} < 1 \\ 0, & \text{if } \dfrac{g_n}{g_{nc}} \geq 1 \end{cases}}$$

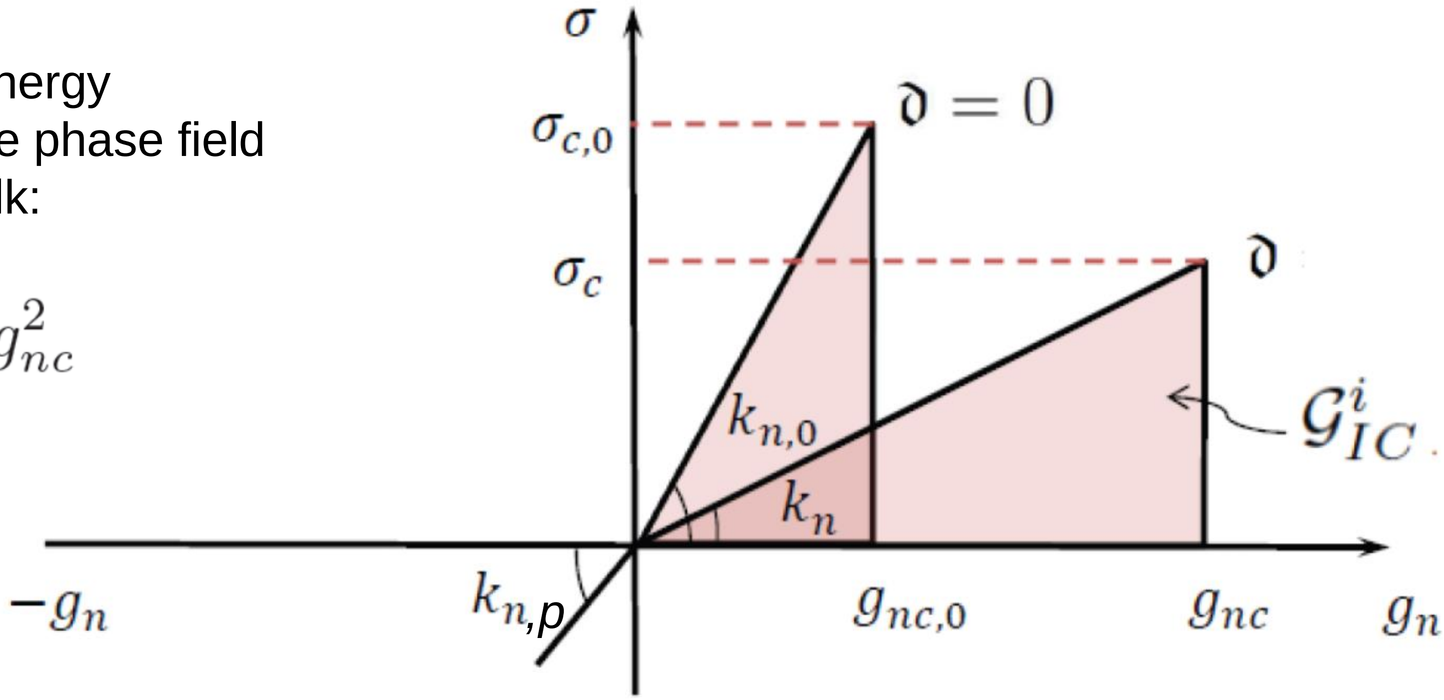
$$g_{nc}(\mathfrak{d}) = (1 - \mathfrak{d})g_{nc,0} + \mathfrak{d}g_{nc,1}$$

$$g_{nc,0} = g_{nc}(\mathfrak{d} = 0)$$

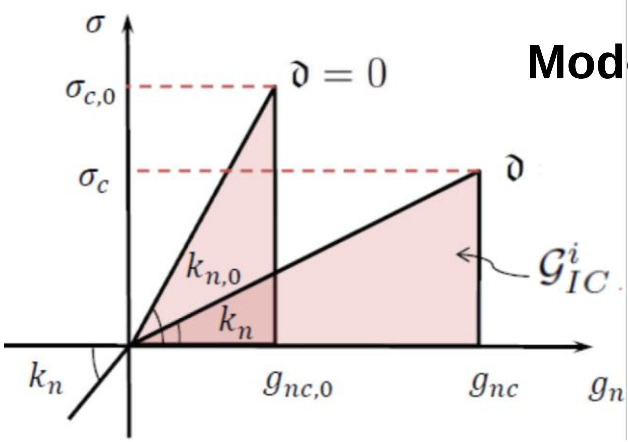
$$g_{nc,1} = g_{nc}(\mathfrak{d} = 1)$$

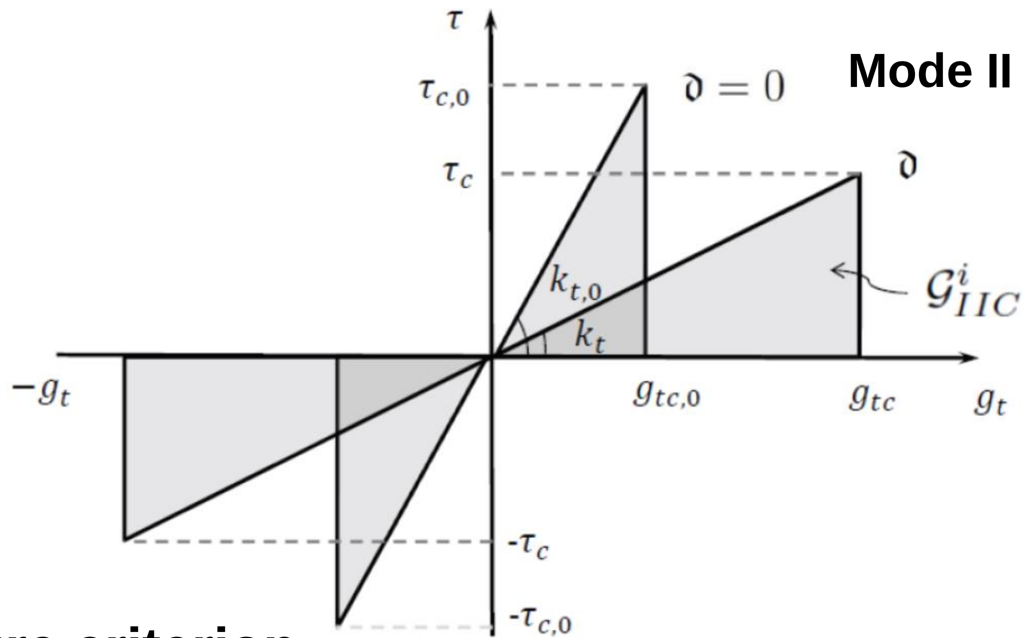
Mode I fracture energy independent of the phase field damage in the bulk:

$$\mathcal{G}_{IC}^i = \frac{1}{2} k_n g_{nc}^2$$



(2) Cohesive Zone Model for interfaces





Energy release rates and fracture criterion:

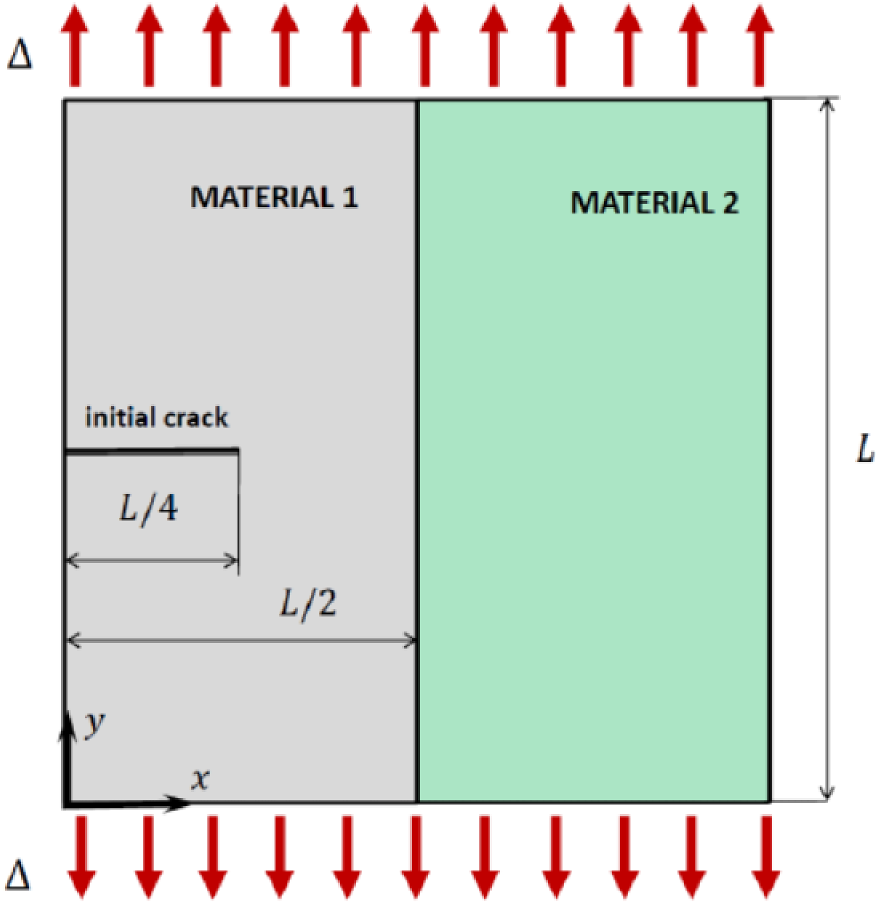
$$\left.\begin{aligned}\mathcal{G}^i_I(\mathfrak{d}) &= \frac{1}{2}k_{n,0}g_n^2\frac{g_{nc,0}^2}{\left[(1-\mathfrak{d})g_{nc,0}+\mathfrak{d}g_{nc,1}\right]^2}\\ \mathcal{G}^i_{II}(\mathfrak{d}) &= \frac{1}{2}k_{t,0}g_t^2\frac{g_{tc,0}^2}{\left[(1-\mathfrak{d})g_{tc,0}+\mathfrak{d}g_{tc,1}\right]^2}\end{aligned}\right\} \quad \left(\frac{\mathcal{G}^i_I}{\mathcal{G}^i_{IC}}\right)^2+\left(\frac{\mathcal{G}^i_{II}}{\mathcal{G}^i_{IIC}}\right)^2=1$$

Test problem: crack perpendicular to a bi-material interface

Dundurs' parameters:

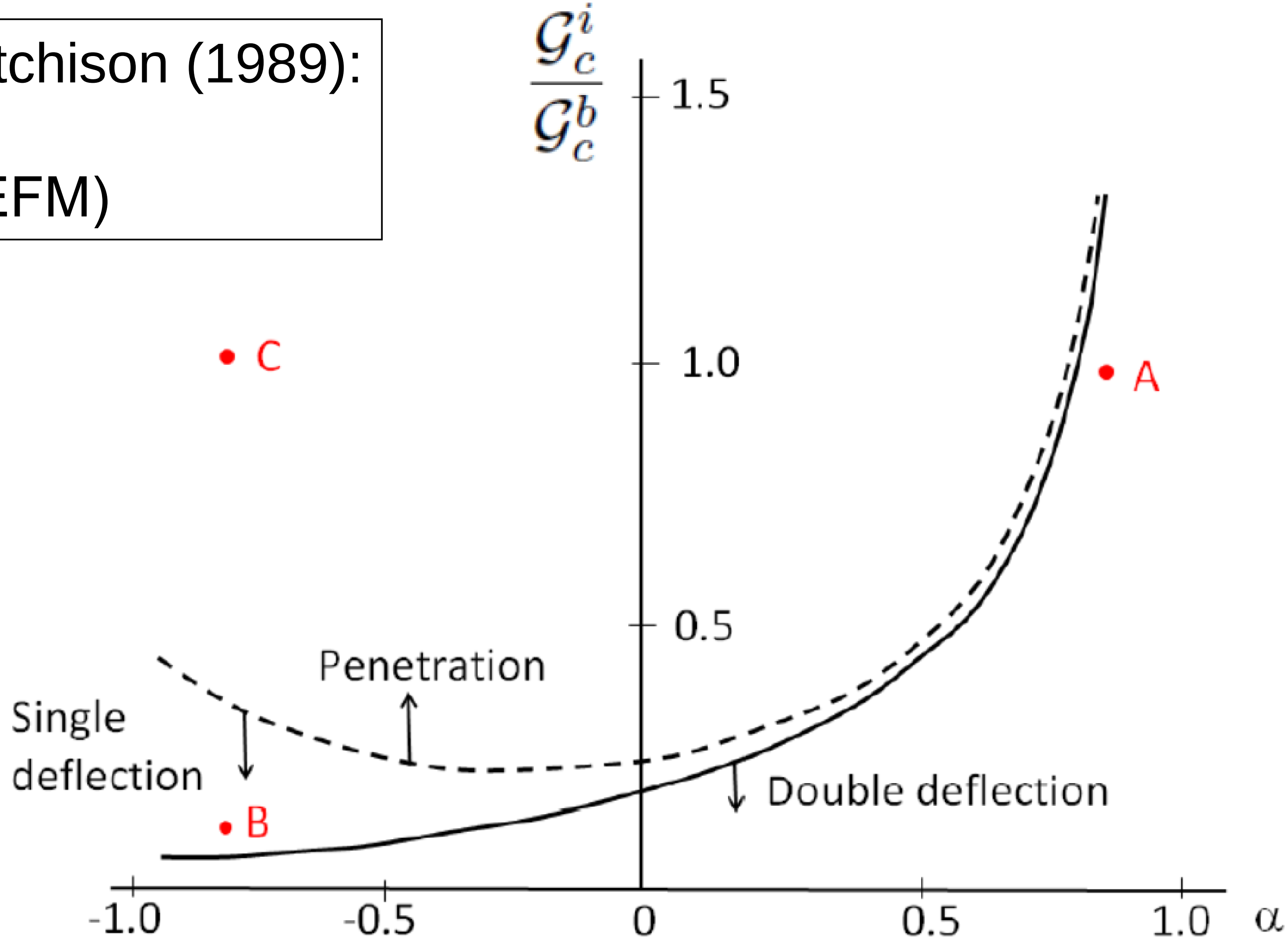
$$\alpha = \frac{\mu_1(1-\nu_2) - \mu_2(1-\nu_1)}{\mu_1(1-\nu_2) + \mu_2(1-\nu_1)}$$

$$\beta = \frac{\mu_1(1-2\nu_2) - \mu_2(1-2\nu_1)}{\mu_1(1-\nu_2) + \mu_2(1-\nu_1)}$$

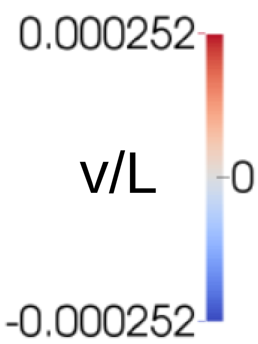


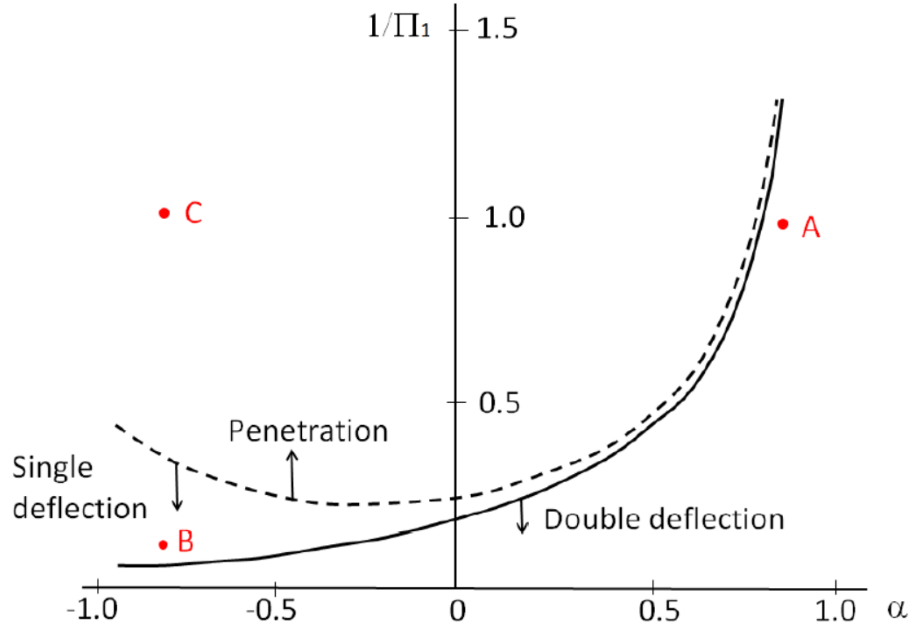
LEFM benchmark

He and Hutchison (1989):
β=0
$l_{CZM}\rightarrow$0 (LEFM)

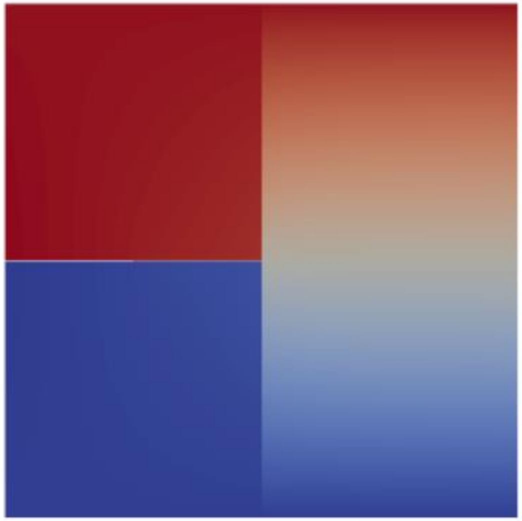


LEFM benchmark

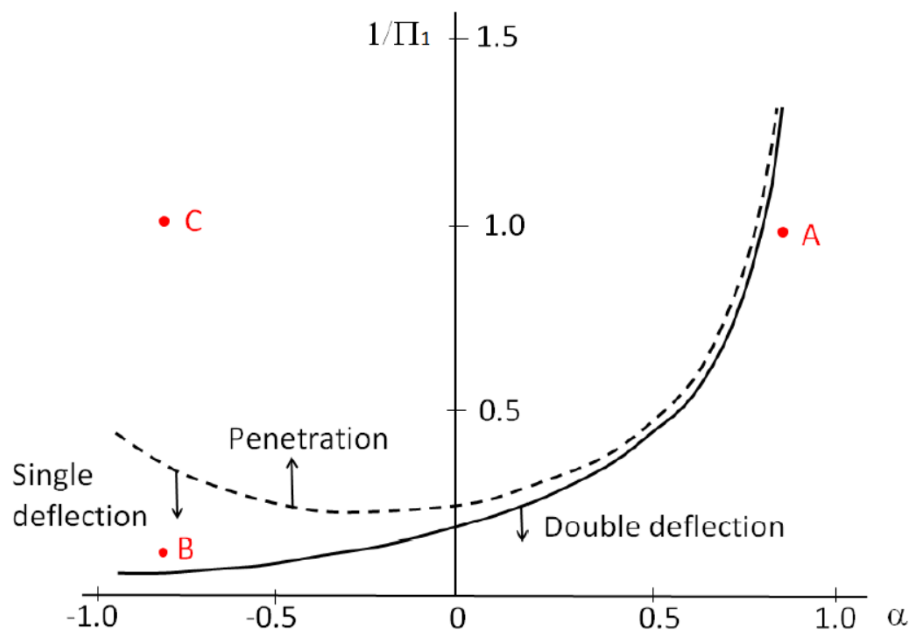




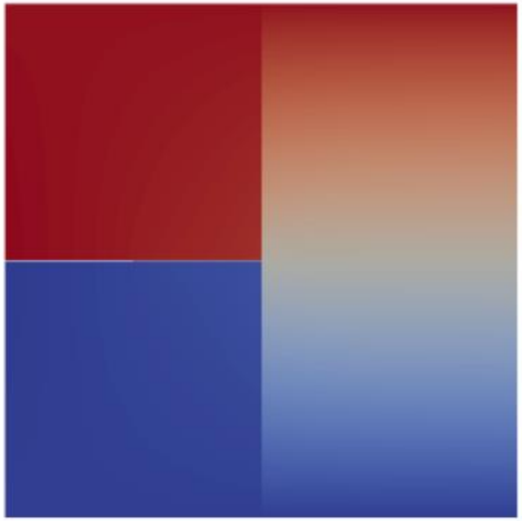
LEFM benchmark



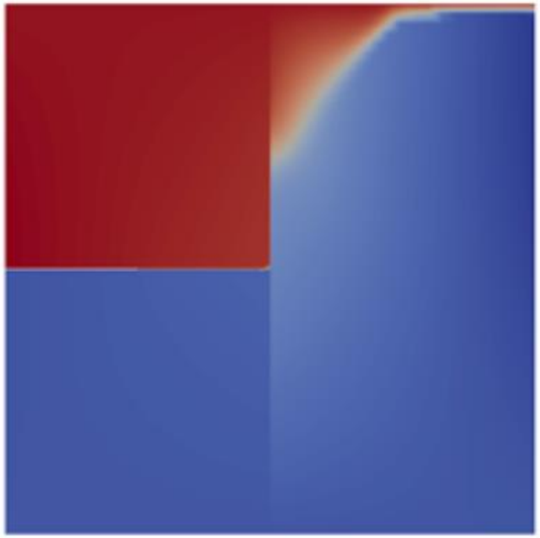
(A)



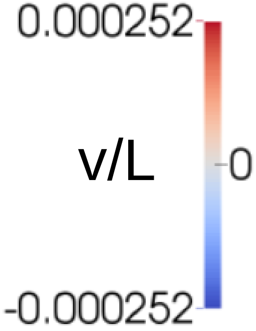
LEFM benchmark

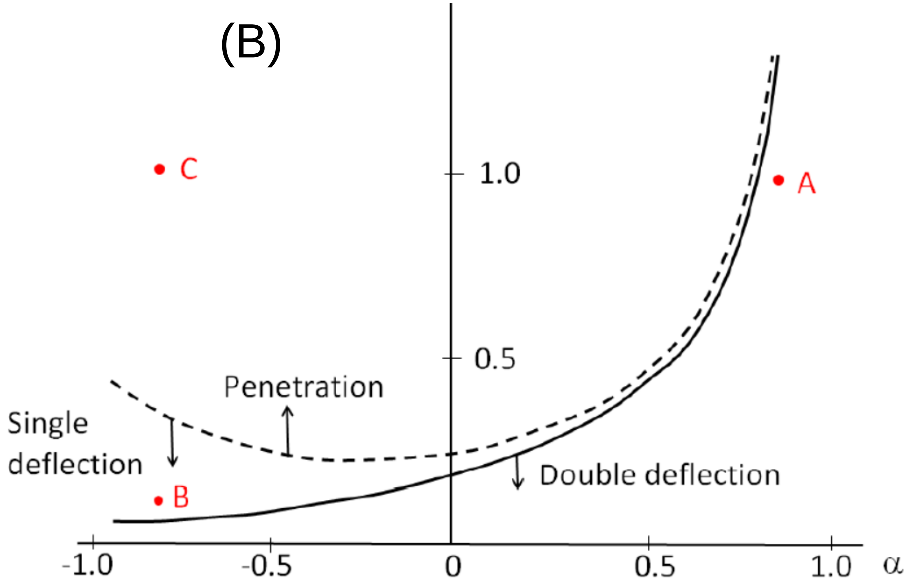


(A)

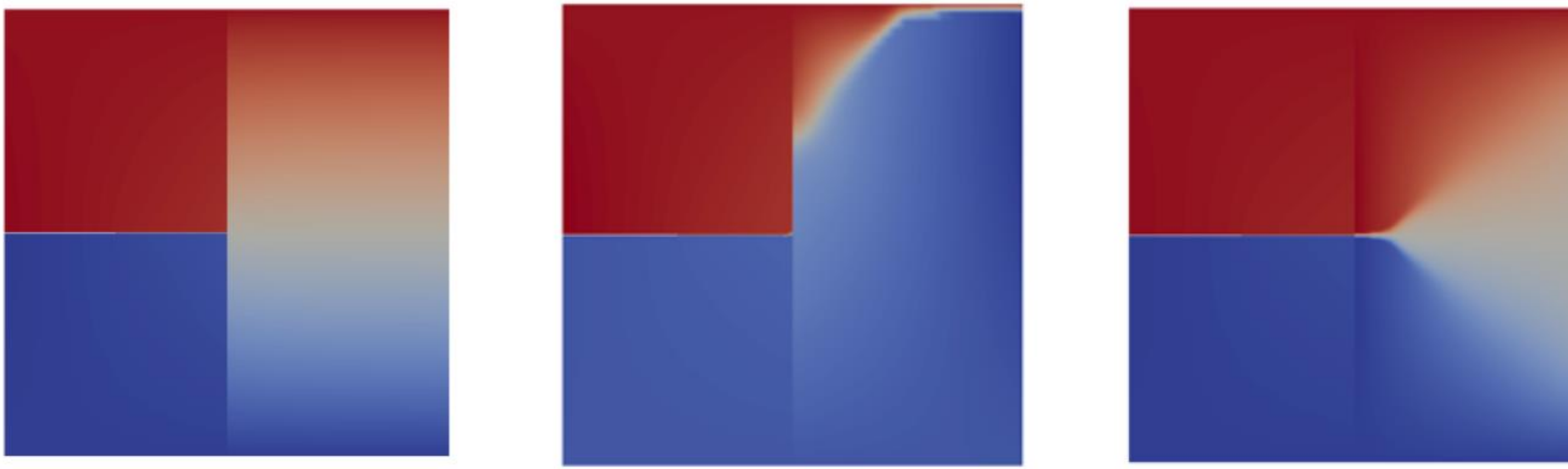


(B)

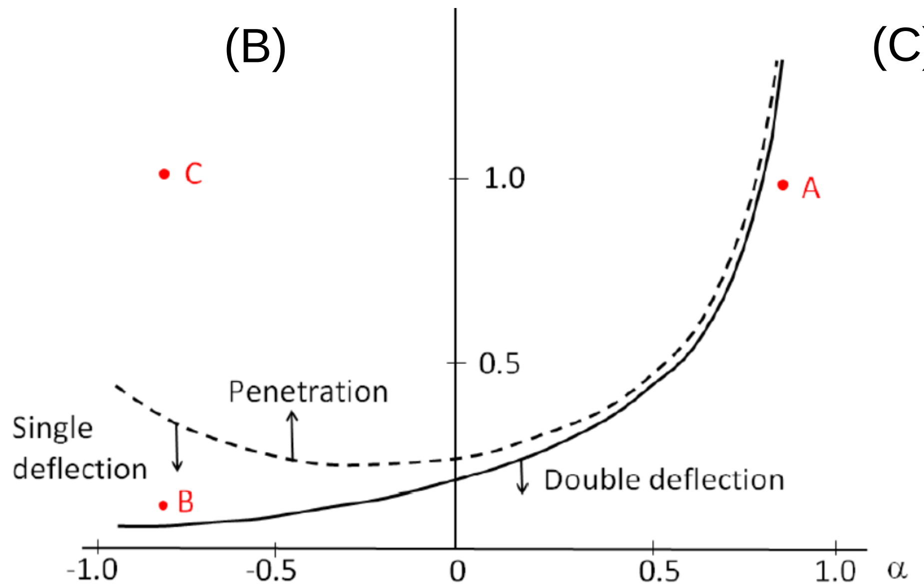




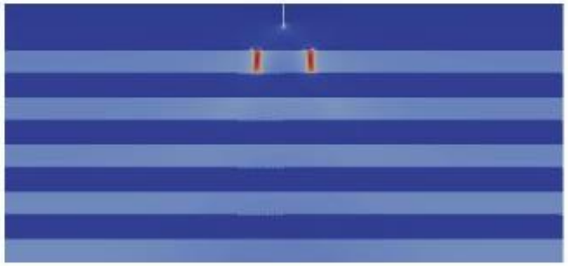
LEFM benchmark



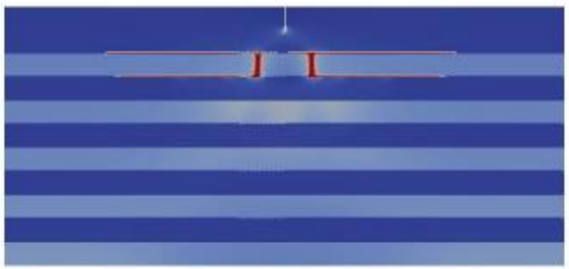
(A) (B) (C)



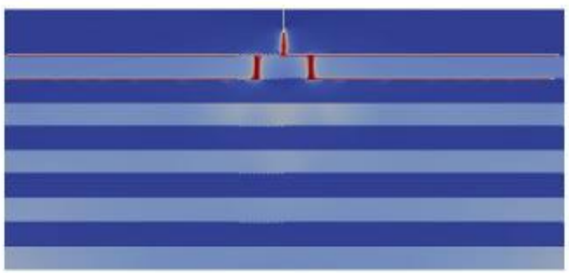
Interlaminar vs. translaminar crack growths



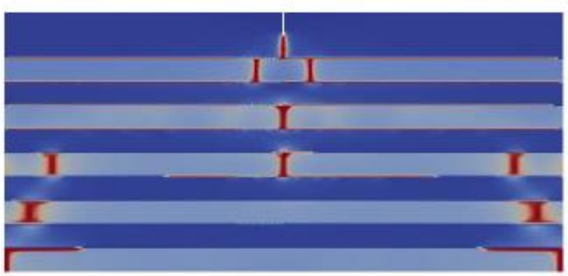
(a)



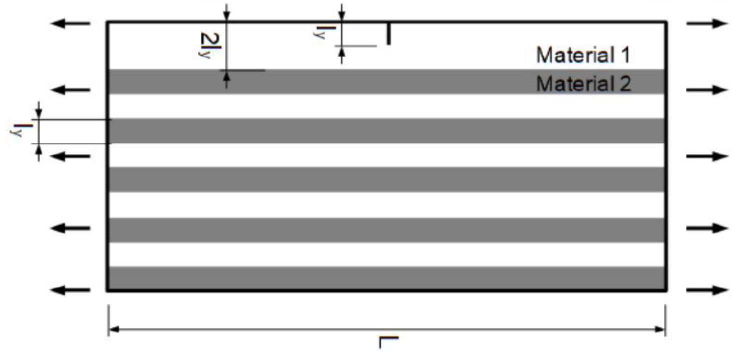
(b)

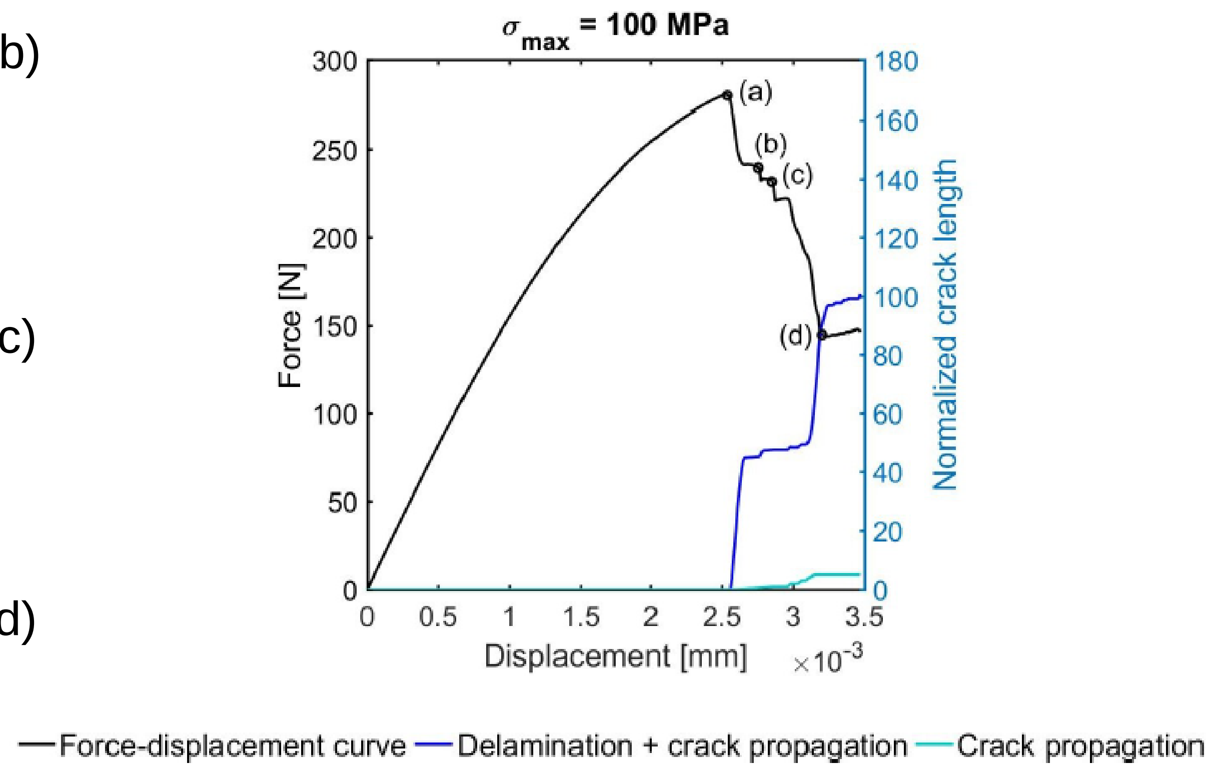


(c)

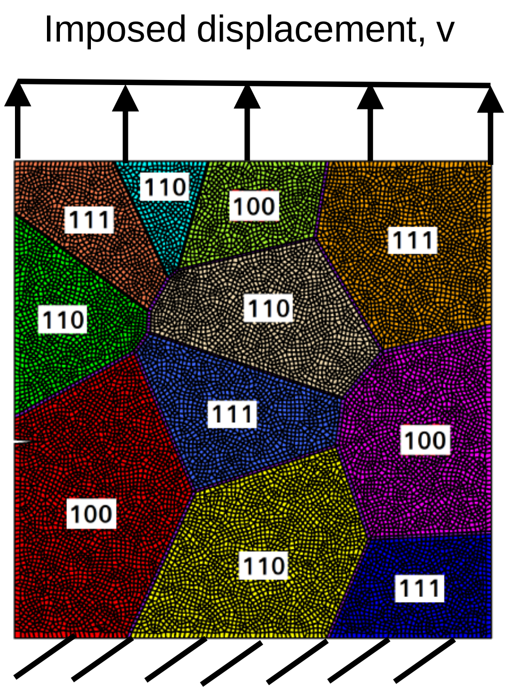


(d)

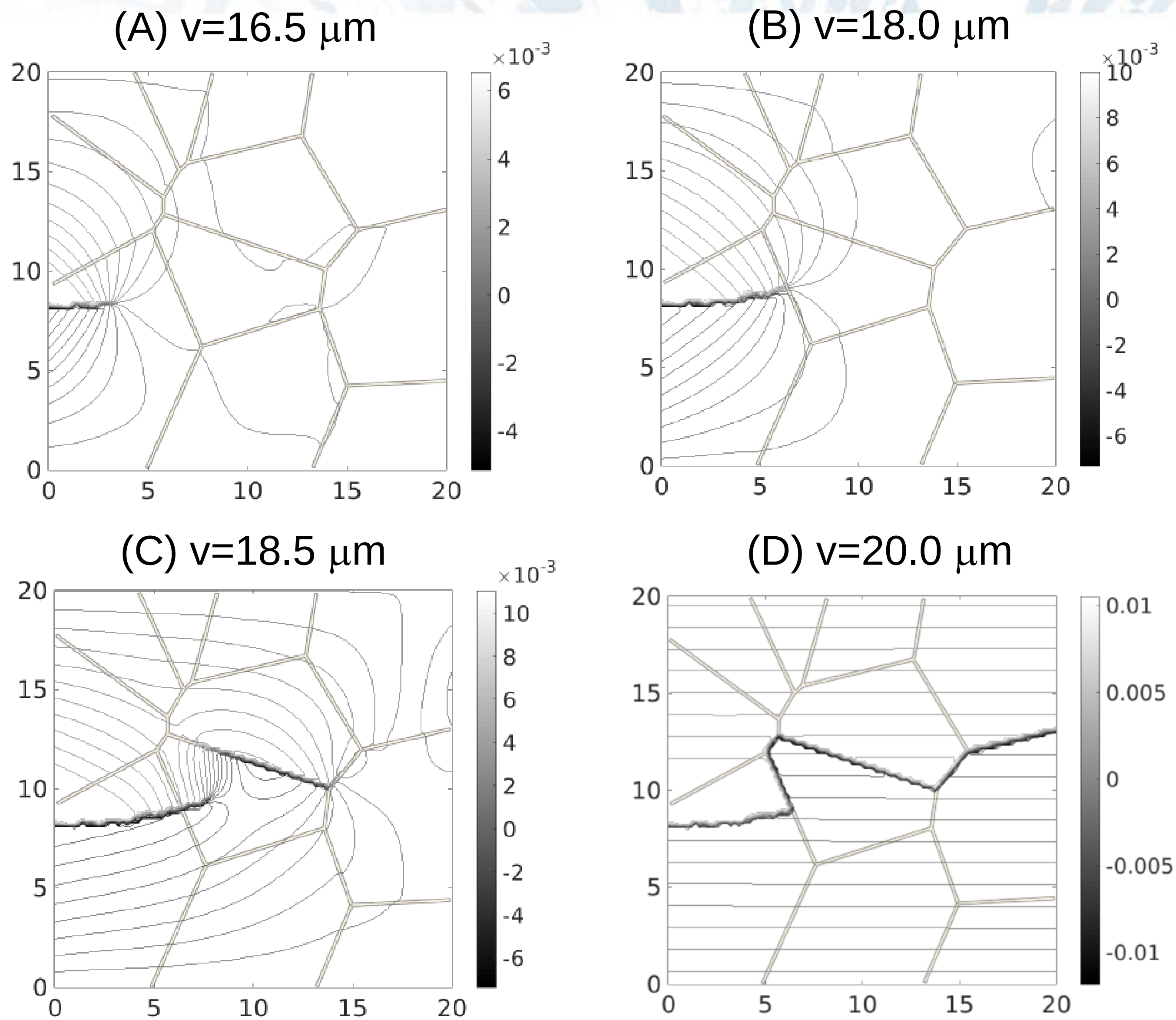




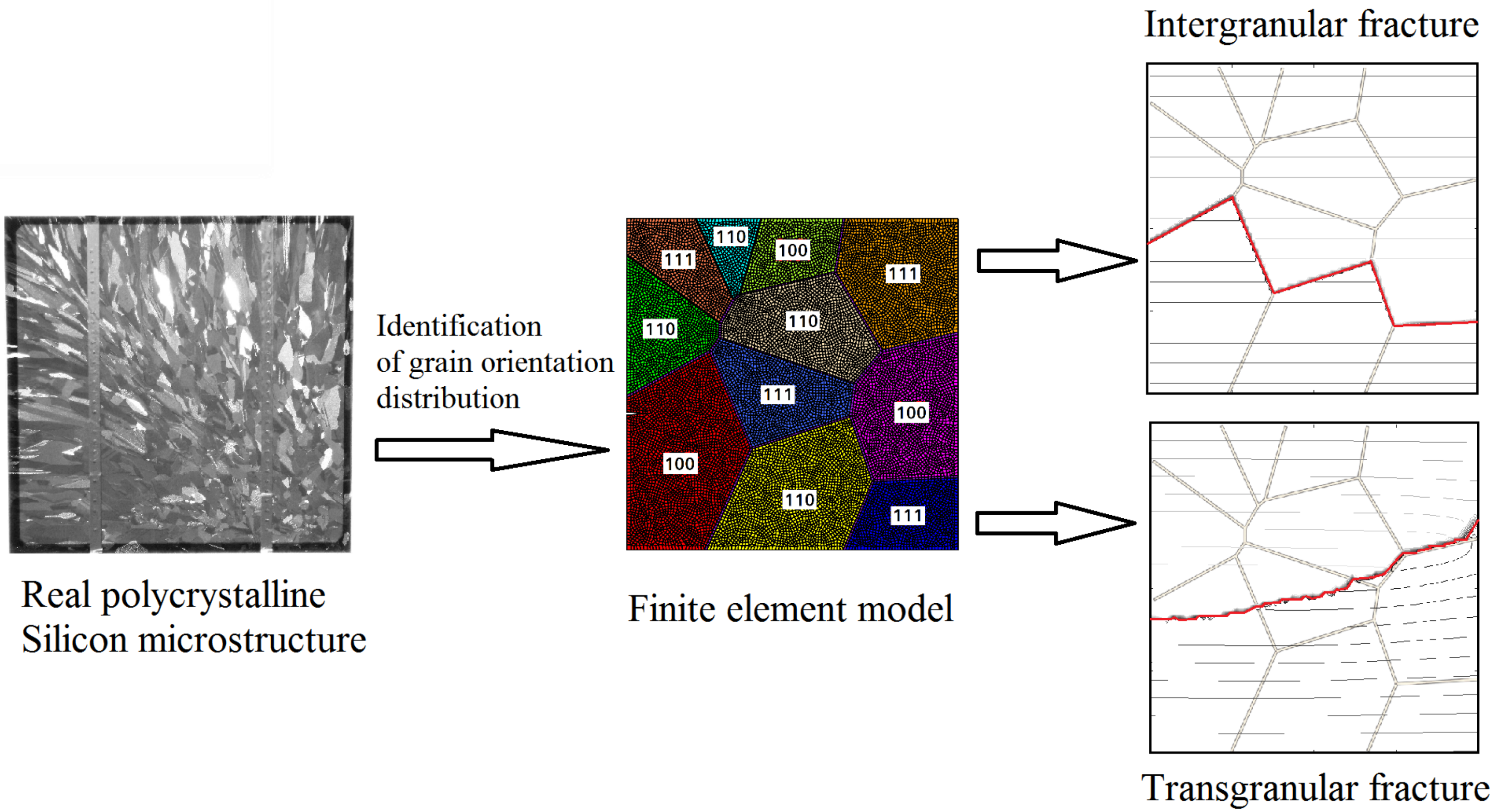
Fracture in anisotropic poly-Silicon



- Anisotropic constitutive tensor for the polycrystals
- Fracture toughness of the grains dependent on their orientation



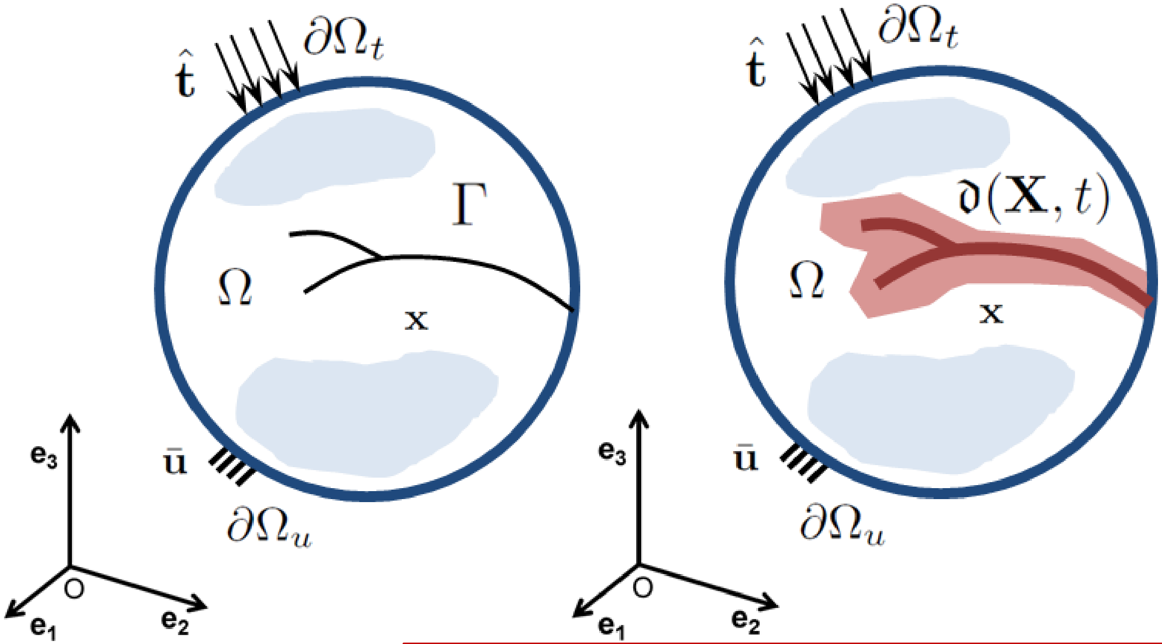
Intergranular vs. transgranular crack growths



M. Paggi, M. Corrado, J. Reinoso (2018) Fracture of solar-grade anisotropic polycrystalline Silicon: A combined phase field–cohesive zone model approach, Computer Methods in Applied Mechanics and Engineering, 330:123-148.

Phase field modeling of fracture in shells

Brittle fracture in solids modeled via a nonlocal smeared crack approach



Phase-field

$$\mathfrak{d}(\mathbf{X}, t) \in [0, 1]$$

Intact **Fully damaged**

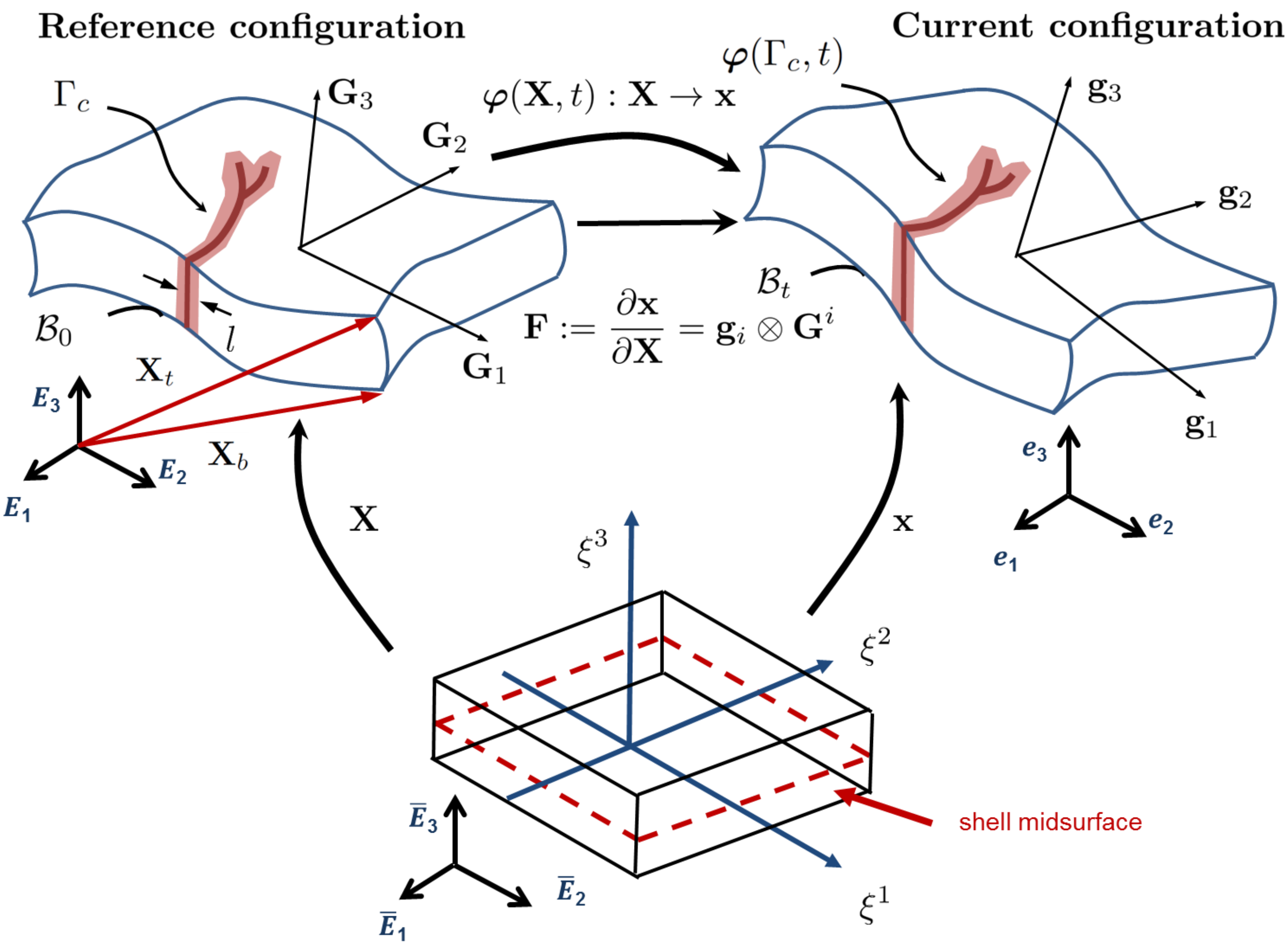
Miehe et al. [2010]]

Potential energy of the body

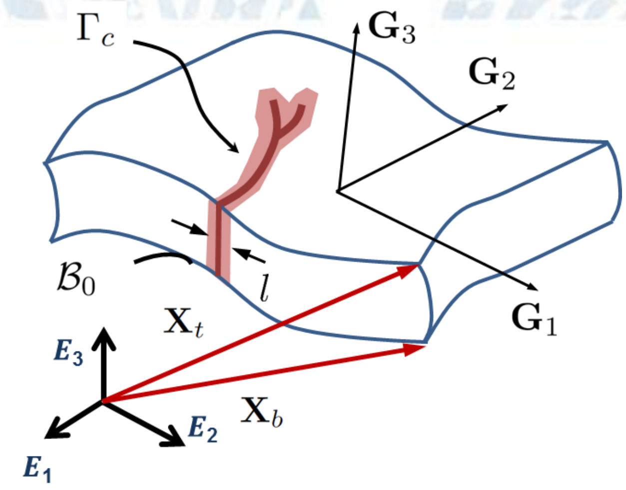
$$\boxed{\Pi(\mathbf{u}, \Gamma) = \underbrace{\int_{\Omega} \psi(\boldsymbol{\varepsilon}) \mathrm{d}\Omega}_{\text{Elastic strain energy}} + \underbrace{\int_{\Gamma_c} \mathcal{G}_c \mathrm{d}\partial\Omega}_{\text{Fracture energy} \rightarrow \text{Griffith approach}}}$$

Miehe, C., Hofacker, M., Welschinger F. (2010) A phase field model for rate independent crack propagation: robust algorithmic implementation based on operator splits. Comput. Methods Appl. Mech. Engrg. 199(45-48):2765--2778.

Phase field modeling of fracture in shells



Phase field modeling of fracture in shells



Geometry interpolation

$$\mathbf{X}(\boldsymbol{\xi}) = \frac{1}{2}\left(1+\xi^3\right)\mathbf{X}_t(\xi^1,\xi^2) + \frac{1}{2}\left(1-\xi^3\right)\mathbf{X}_b(\xi^1,\xi^2)$$

Phase field interpolation

$$\mathfrak{d}(\xi^1,\xi^2,\xi^3) = \frac{1}{2}\left(1+\xi^3\right)\mathfrak{d}_t(\xi^1,\xi^2) + \frac{1}{2}\left(1-\xi^3\right)\mathfrak{d}_b(\xi^1,\xi^2)$$

Variational form including the EAS method to prevent locking

$$\Pi(\mathbf{S},\tilde{\mathbf{E}},\mathbf{u},\mathfrak{d}) = \int_{\mathcal{B}_0} \mathfrak{g}(\mathfrak{d})\Psi(\mathbf{E}^u,\tilde{\mathbf{E}})\,\mathrm{d}\Omega - \int_{\mathcal{B}_0} \mathbf{S}:\tilde{\mathbf{E}}\,\mathrm{d}\Omega + \int_{\mathcal{B}_0} \frac{\mathcal{G}_c l}{2}\left(\frac{\mathfrak{d}^2}{l^2} + |\nabla_{\mathbf{X}}\mathfrak{d}|^2\right)\mathrm{d}\Omega + \Pi_{\mathrm{ext}}$$

$$\overline{\Psi}(\mathbf{E}^u,\tilde{\mathbf{E}},\mathfrak{d}) = \mathfrak{g}(\mathfrak{d})\Psi(\mathbf{E}^u,\tilde{\mathbf{E}}), \quad \text{with} \quad \mathfrak{g}(\mathfrak{d}) = [1-\mathfrak{d}]^2 + \mathcal{K}$$

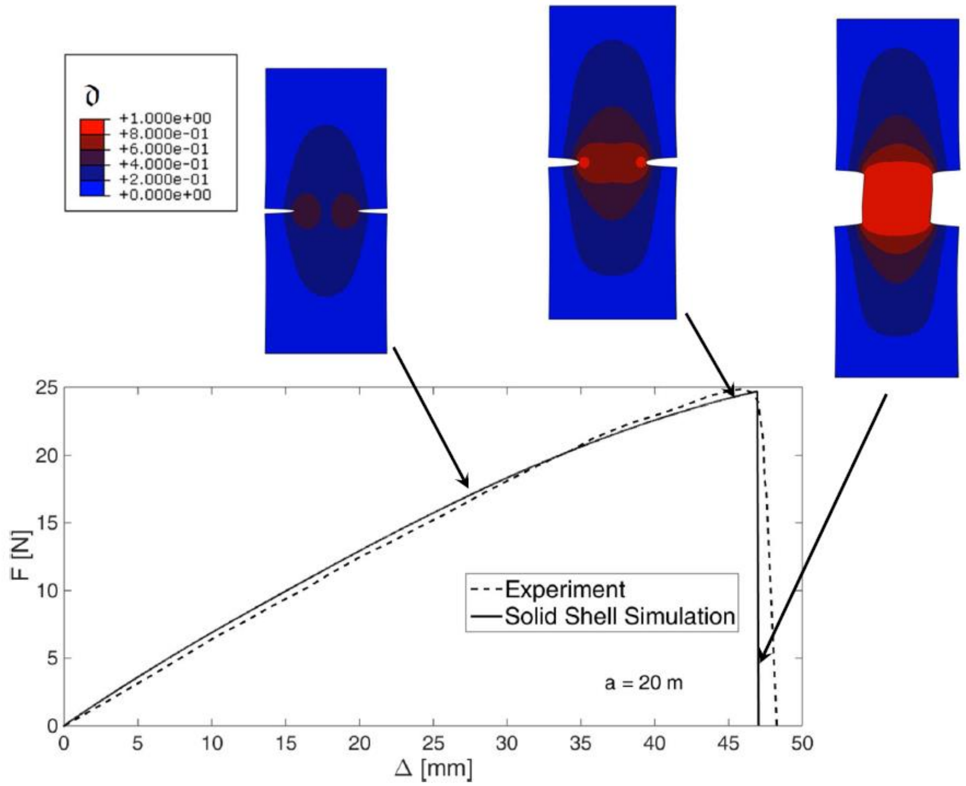
Phase-field stiffness degradation

Intact free energy accounting for incompatible strains

- **Poisson thickness locking**
  Unmodified 3D material laws
- **Volumetric locking**

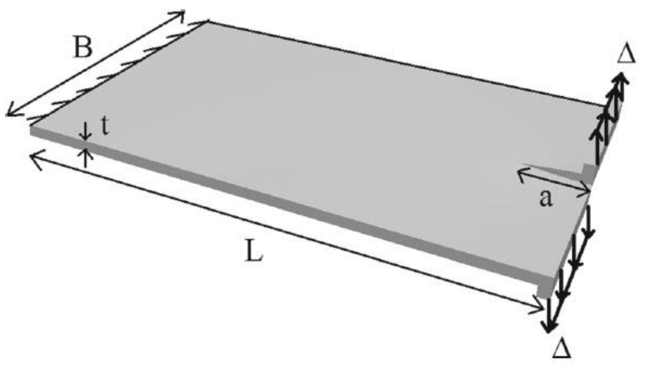
Phase field modeling of fracture in shells

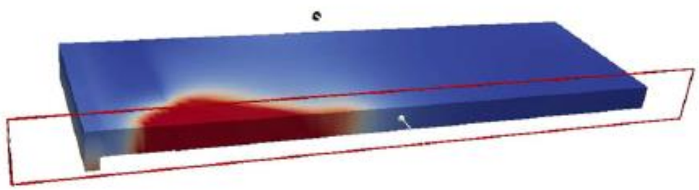
- Monolithic and fully implicit formulation
- Phase field interpolation through the shell thickness
- ANS + EAS technologies (for Poisson thickness and volumetric locking pathologies)
- Linear elastic and nonlinear elastic constitutive relations
- FEAP & Abaqus implementation

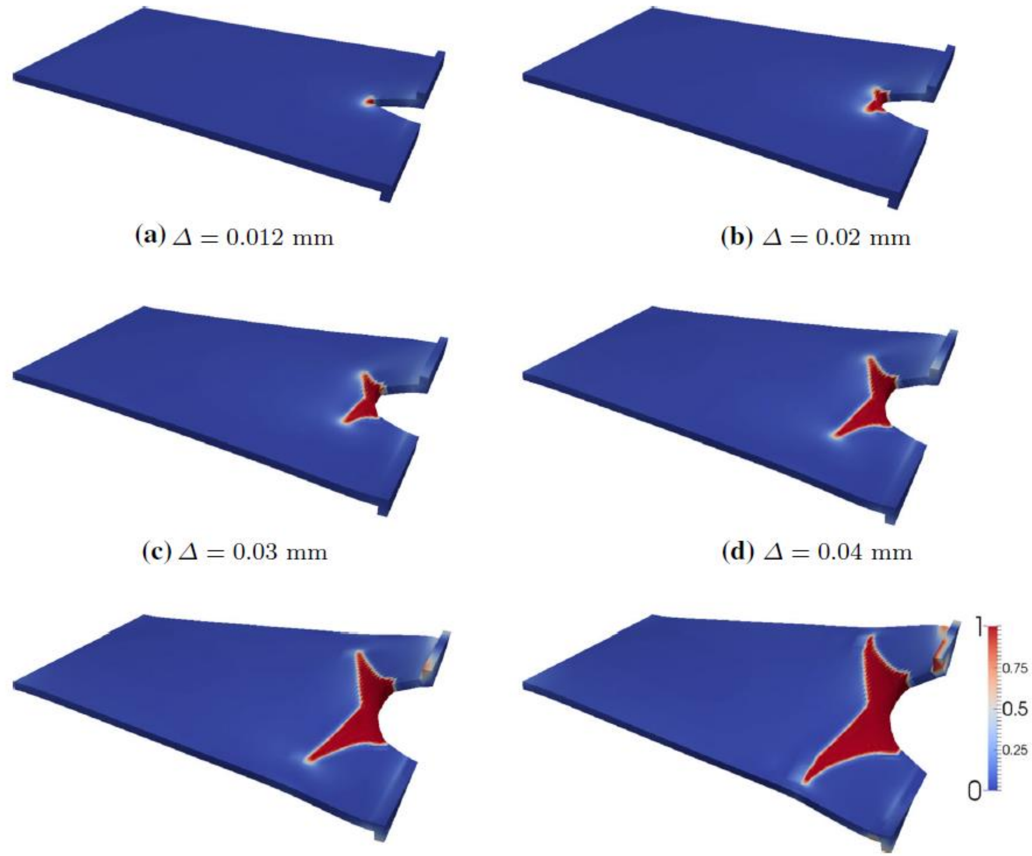


J. Reinoso, M. Paggi, C. Linder (2017) Phase field modeling of brittle fracture for enhanced assumed strain shells at large deformations: formulation and finite element implementation, **Computational Mechanics**, DOI 10.1007/s00466-017-1386-3

Phase field modeling of fracture in shells



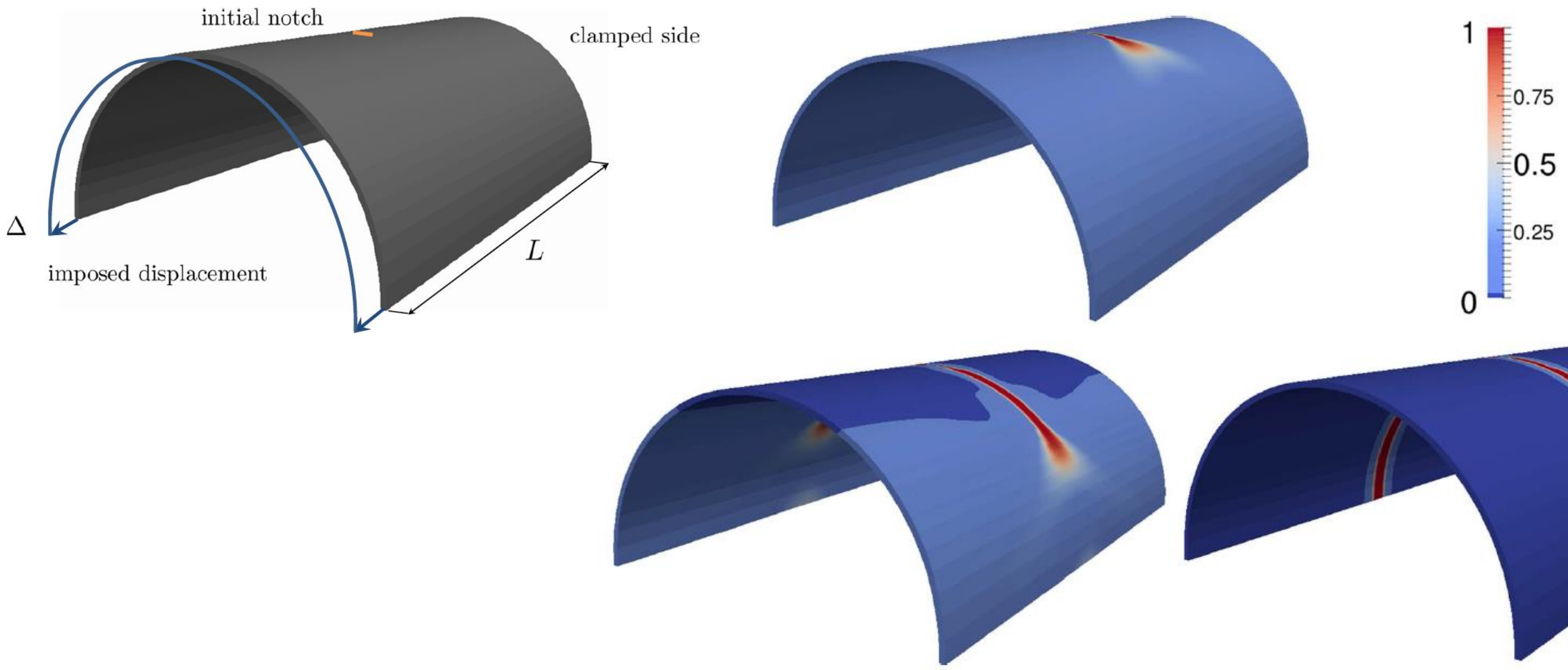




(a) $\Delta = 0.012$ mm
(b) $\Delta = 0.02$ mm
(c) $\Delta = 0.03$ mm
(d) $\Delta = 0.04$ mm
(e) $\Delta = 0.05$ mm
(f) $\Delta = 0.064$ mm

J. Reinoso, M. Paggi, C. Linder (2017) Phase field modeling of brittle fracture for enhanced assumed strain shells at large deformations: formulation and finite element implementation, **Computational Mechanics**, DOI 10.1007/s00466-017-1386-3

Phase field modeling of fracture in shells



J. Reinoso, M. Paggi, C. Linder (2017) Phase field modeling of brittle fracture for enhanced assumed strain shells at large deformations: formulation and finite element implementation, **Computational Mechanics**, DOI 10.1007/s00466-017-1386-3

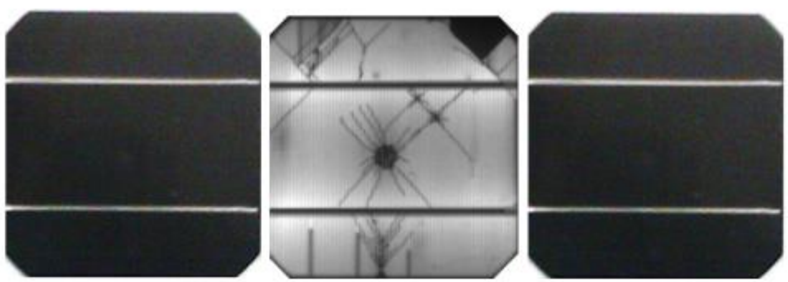
IMT SCUOLA ALTI STUDI LUCCA

Acknowledgements

http://musam.imtlucca.it

https://www.facebook.com/fanpagemusam

Multi-field and multi-scale Computational Approach to design and durability of Photovoltaic Modules – CA2PVM



erc European Research Council Established by the European Commission

IDEAS