



SCHOOL
FOR ADVANCED
STUDIES
LUCCA



Frontier research on multi-scale analysis of materials

Marco Paggi

IMT School for Advanced Studies Lucca

Laboratorio NEST, Scuola Normale Superiore, Pisa, 30/11/2017

MUSAM –**Multi-scale Analysis of Materials**– is a research unit of the IMT School for Advanced Studies Lucca contributing to research and educational programs by integrating:

- **Numerical analysis**
- **Mechanics (computational and experimental)**
- **Materials science**

for the characterization and simulation of **natural or artificial materials** characterized by **multiple scales** or in the presence of **multiple fields (coupled problems)**

Multi-scale Analysis of Materials

MUSAM Research unit

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

Post-docs

- **C. Borri**
- **M. Gagliardi**

PhD students

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

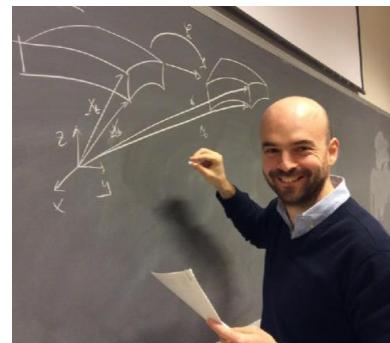
Former staff

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



Visiting professors

- **D. Bigoni**, University of Trento
- **J. Reinoso**, University of Seville
- **M. Corrado**, Politecnico di Torino
- **A. Gizzi**, Università Campus Bio-Medico of Rome
- **A. Popp**, TU Munich
- **A. Vakis**, University of Groningen
- **D. Piga**, SUPSI Lugano



International cooperations

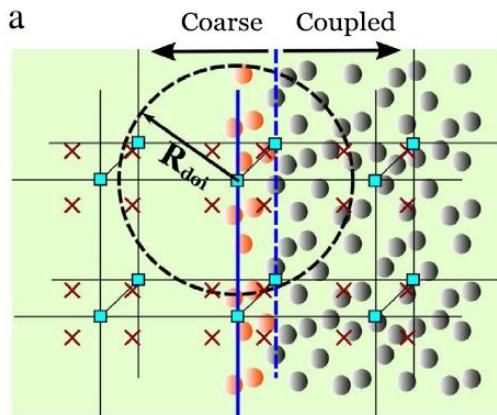
- **C. Linder** Stanford University (LA, USA) 
- **J.R. Barber** University of Michigan (MI, USA) 
- **D.A. Hills** University of Oxford (UK) 
- **F. Borodich** Cardiff University (UK) 
- **P. Wriggers, R. Rolfes** University of Hannover (Germany)
- **R. Brendel, S. Kajari-Schröder** Institute for Solar Energy Research Hamelin (Germany) 
- **T. Rabczuk** Bauhaus University of Weimar (Germany) 
- **V. Popov** TU Berlin (Germany) 
- **Q.-C. He** University of Paris-EST (France) 
- **J. Reinoso, V. Mantic** University of Seville (Spain) 
- **P.P. Camanho** University of Porto (Portugal) 
- **P. Areias** University of Evora (Portugal) 
- **O. Naimark, O. Plekhov** Russian Academy of Sciences (Russia) 

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



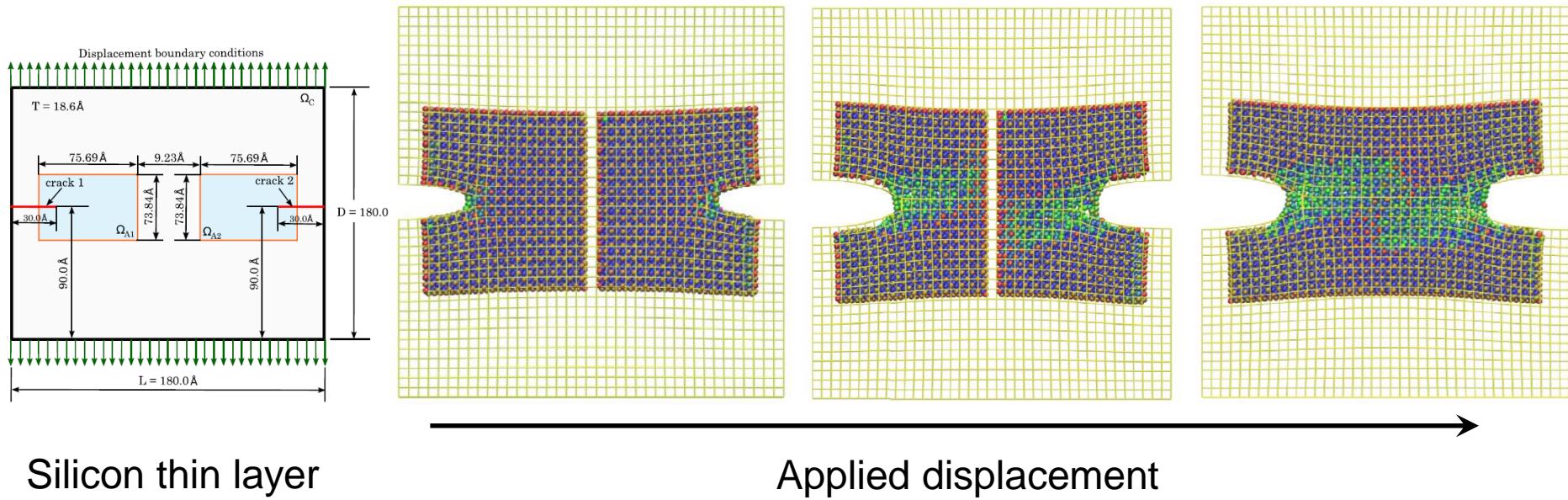
- **3D confocal-interferometric profilometer (LEICA, DCM 3D)**
- **Scanning Electron Microscope (ZEISS, EVO MA15)**
- **Micromechanical testing stage (DEBEN, 5000S)**
- **Universal testing machine with a thermostatic chamber (Zwick/Roell, Z010TH) and a peeling test setup**
- **Thermocamera (FLIR, T640bx)**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

Multiscale computational fracture mechanics

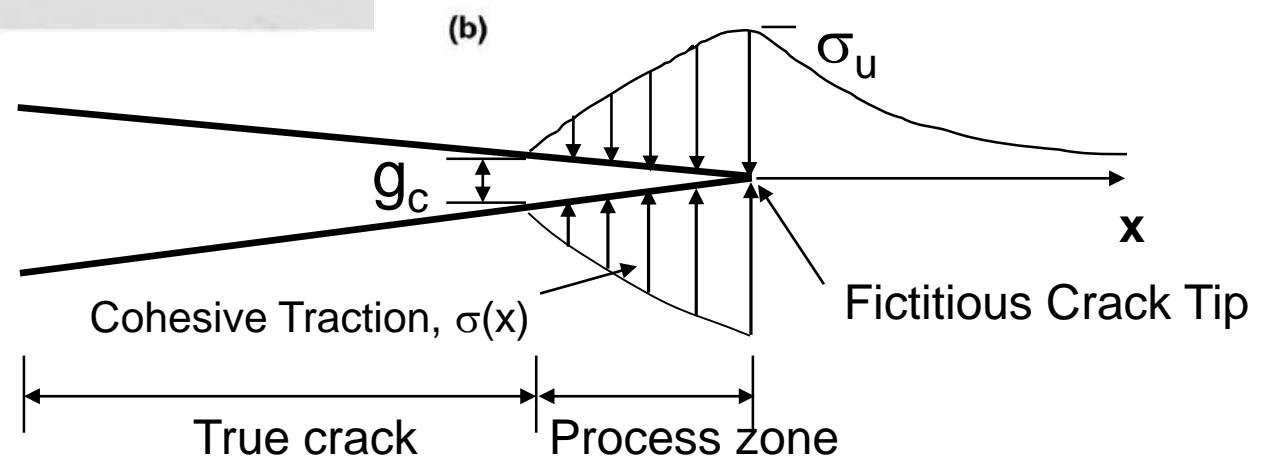
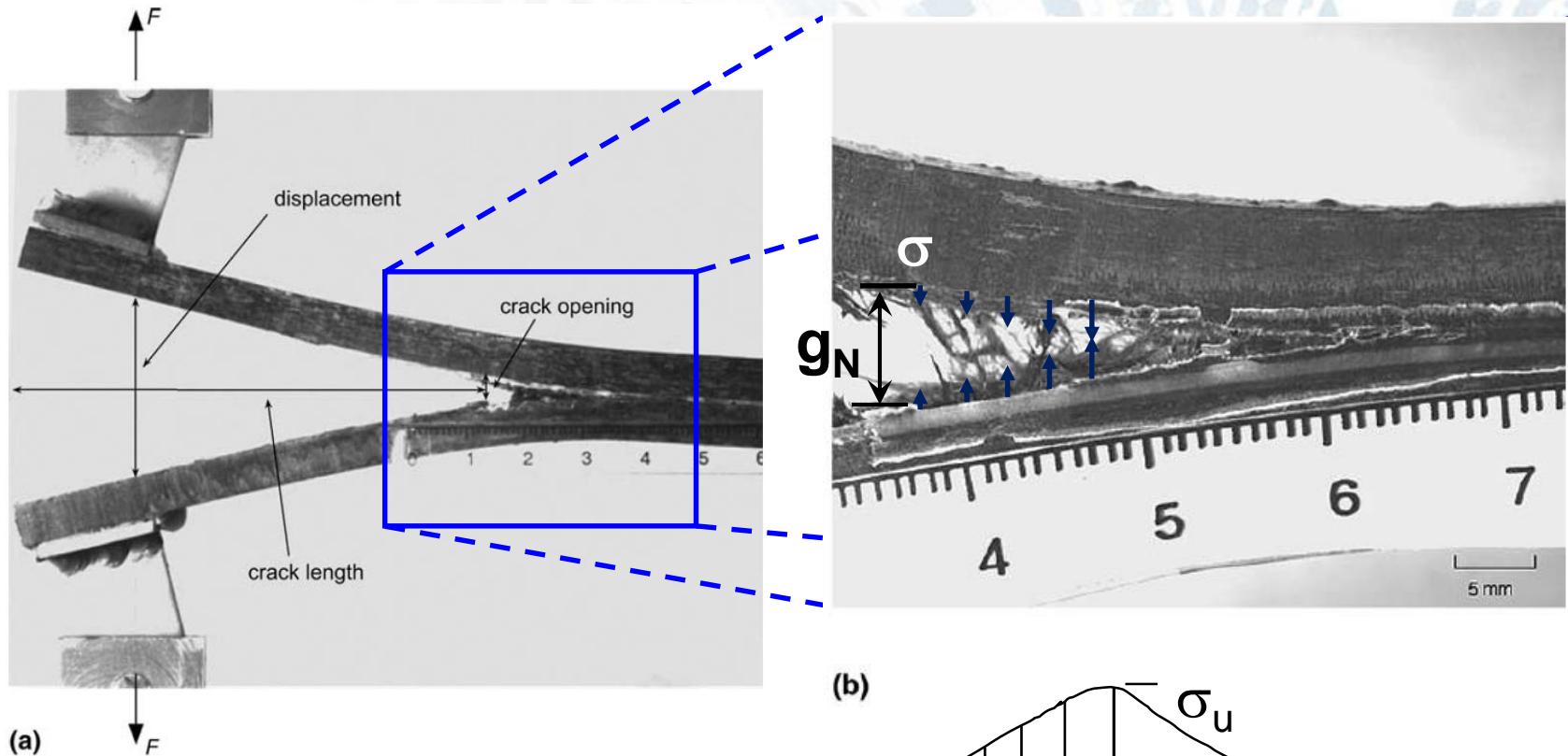


Key features:

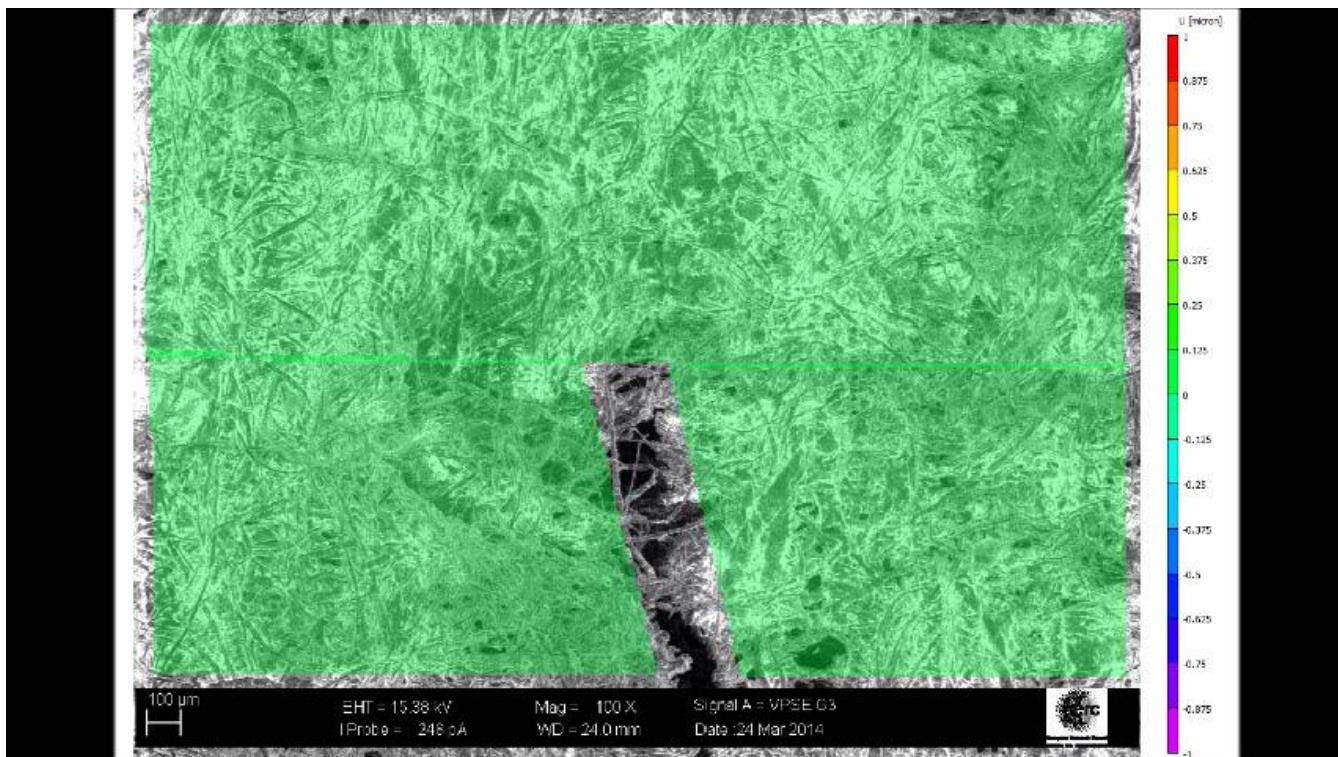
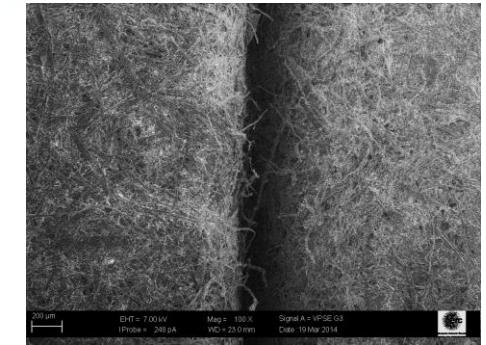
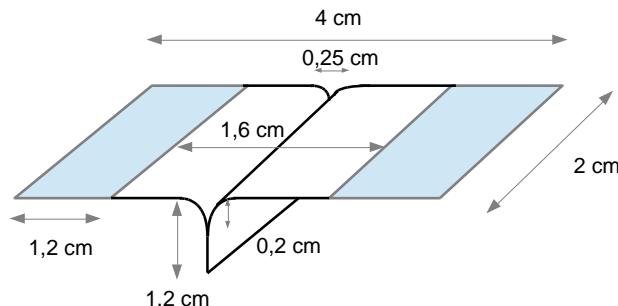
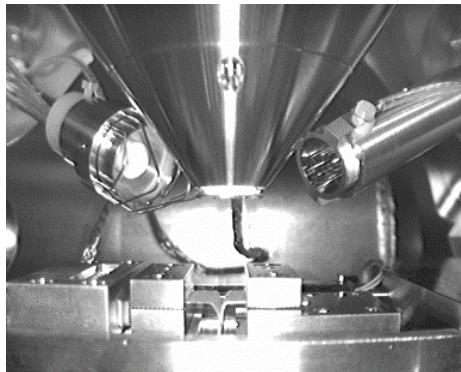
- Concurrently coupled FEM (solid shells with phantom node method) & molecular statics (LAMMPS) model
- Adaptive refinement
- Prediction of crack branching from molecular statics



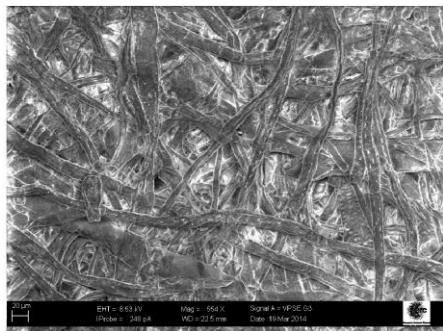
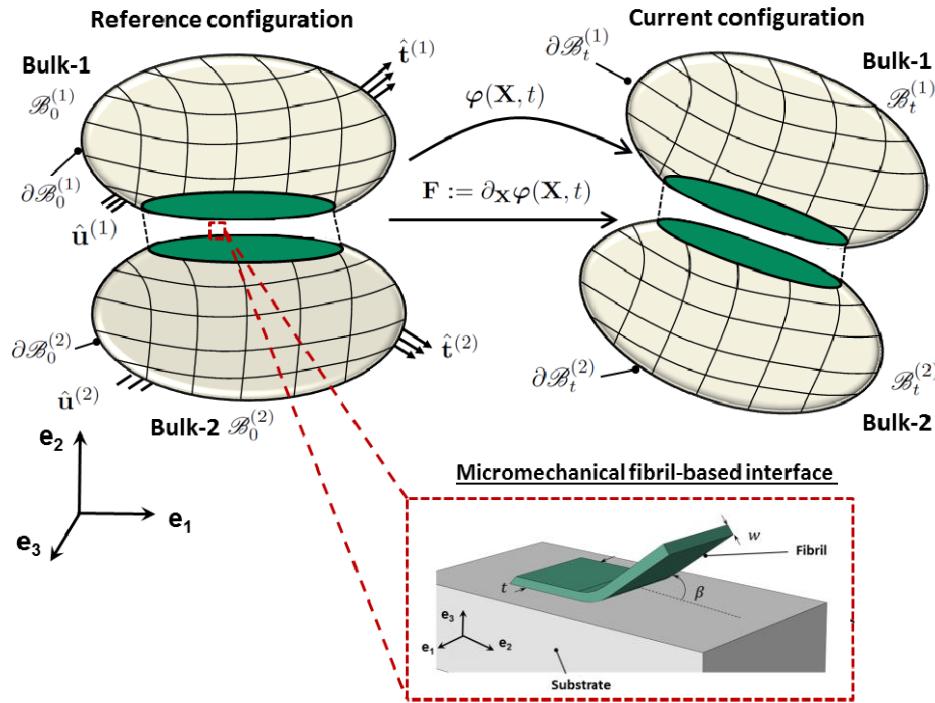
Computational fracture mechanics: fibrous materials



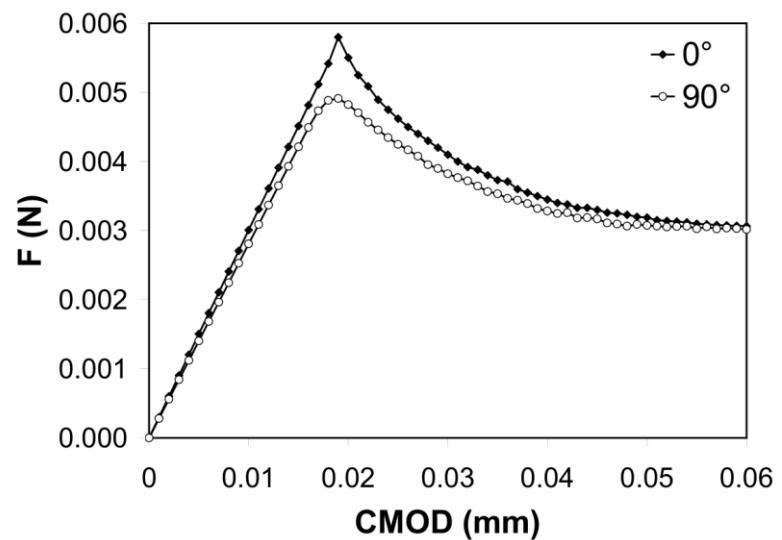
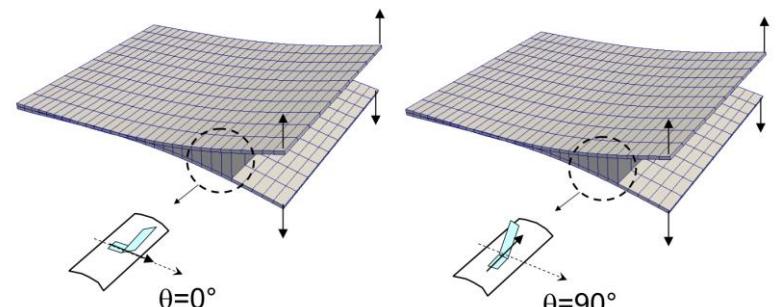
Computational fracture mechanics: fibrous materials



Computational fracture mechanics of fibrous materials



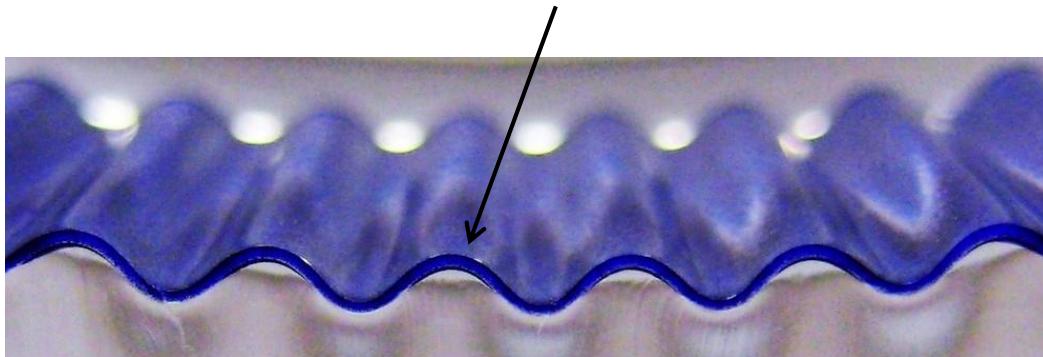
- Key features:**
- Fiber orientation distribution
 - Finite elasticity
 - New finite element



The effect of fiber anisotropy on the peeling resistance

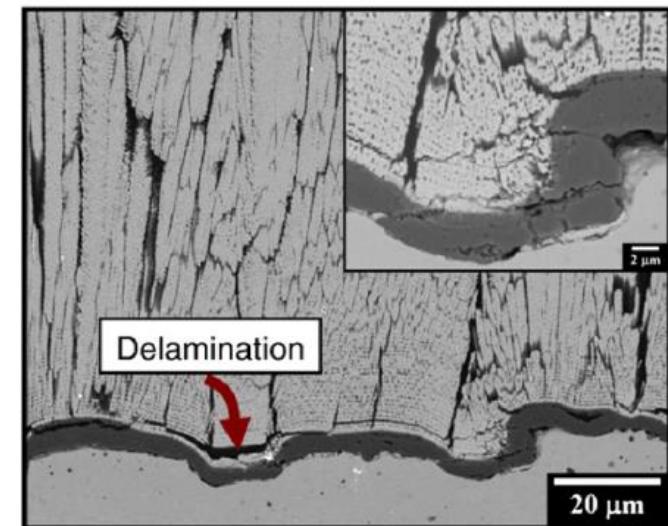
Computational fracture mechanics of coatings: interplay between fracture and instability

Buckling-driven delamination in case of wrinkling



Brau et al. (2011) Multiple-length-scale elastic instability mimics parametric resonance of nonlinear oscillators, Nature Physics 7, 56-60.

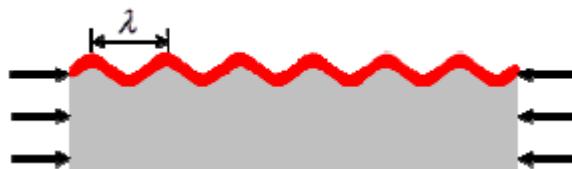
Failure of thermal-barrier coatings



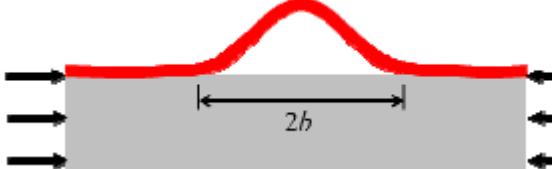
Zhao et al. (2010) Surf. Coat. Tech. 204:2432-2441

Potential multiple scenarios

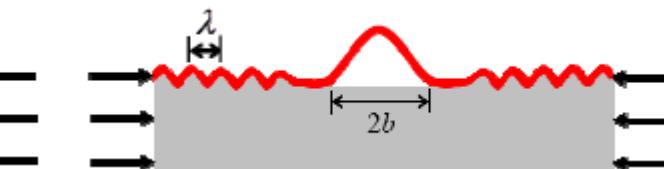
Wrinkling but no delamination



Buckled delamination



Wrinkle-induced delamination

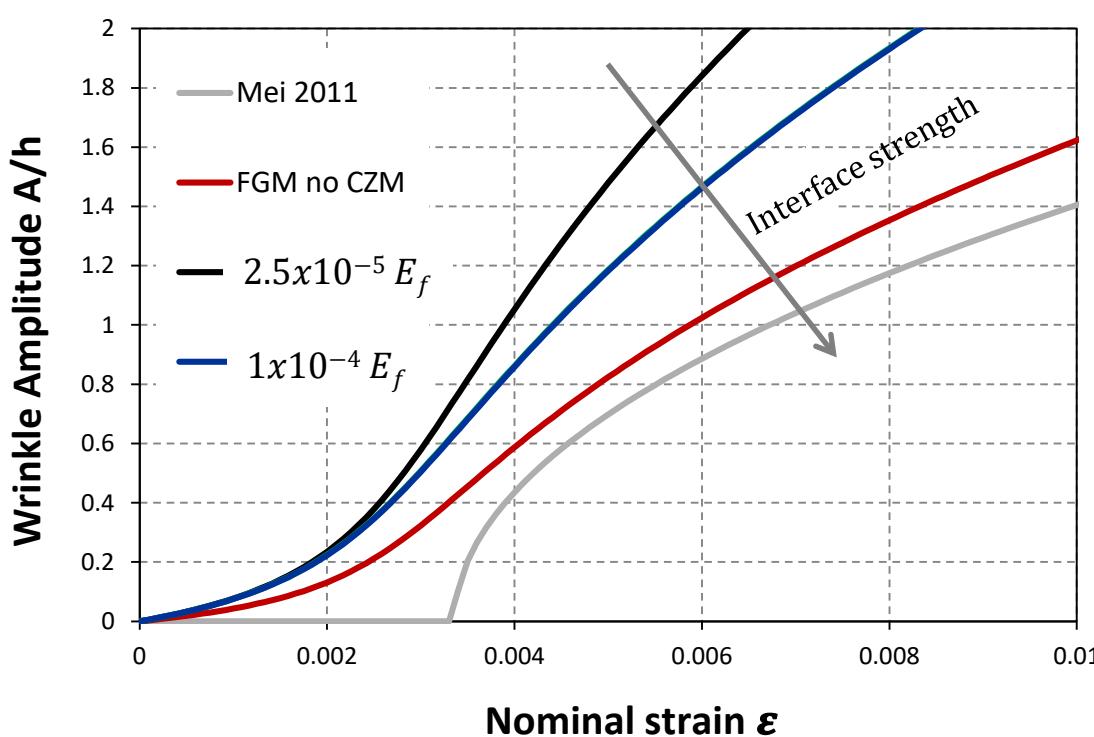


Mei H. (2011) Fracture and delamination of elastic thin films on compliant substrates: modeling and simulations, PhD Dissertation Univ. Texas Austin

Computational fracture mechanics of coatings: interplay between fracture and instability

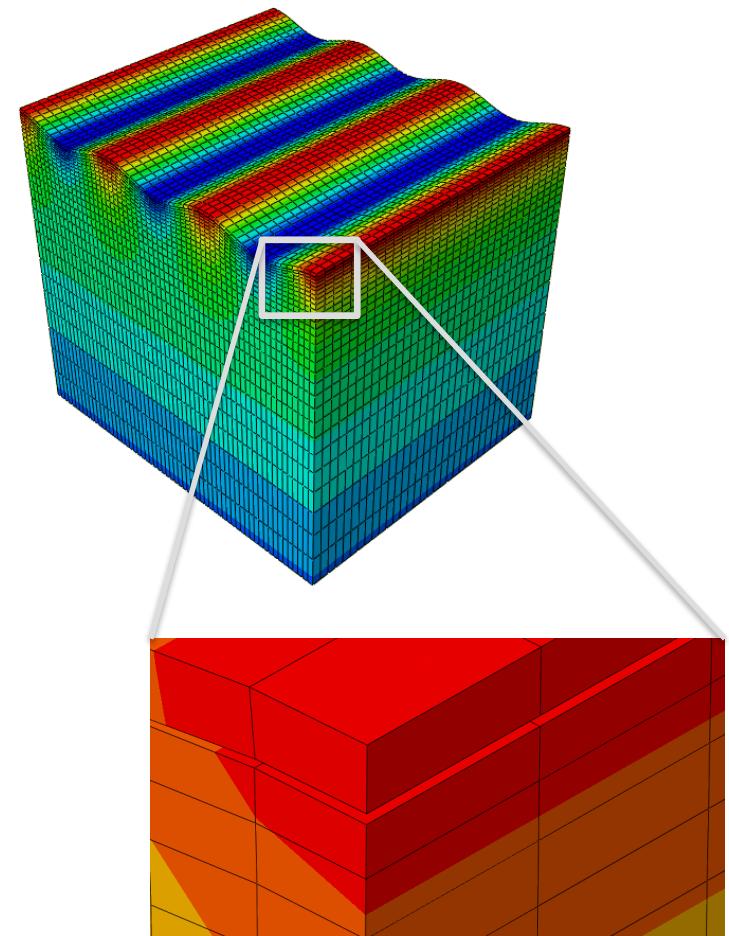
Key features:

- Solid shell finite elements coupled with interface finite elements for the study of the interplay between fracture and geometrical instability

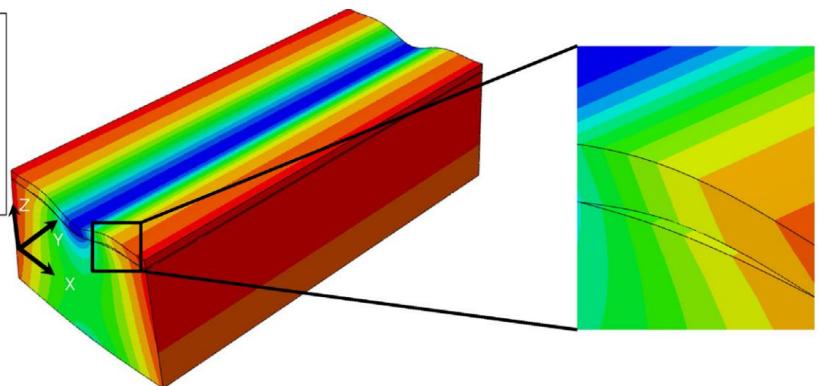
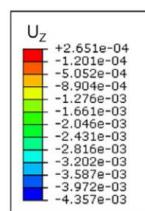
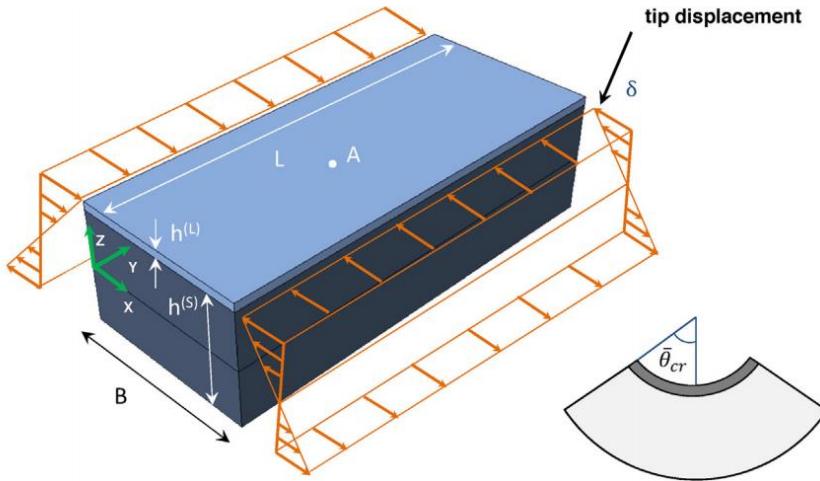


$$A = h \sqrt{\frac{\varepsilon}{\varepsilon_{cr}} - 1}$$

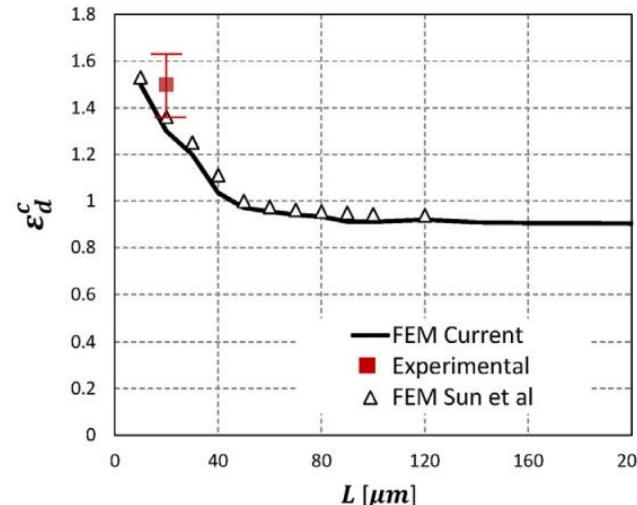
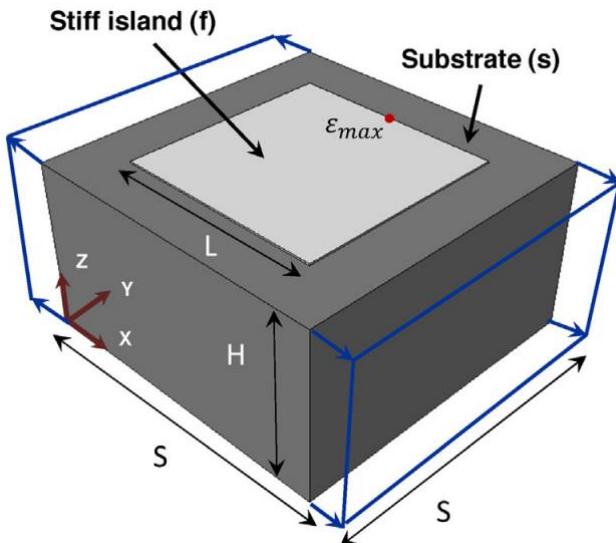
[Wrinkle amplitude \(Mei 2011\)](#)
[based on fully bonded interface and homogeneous layer](#)



Computational fracture mechanics of coatings: interplay between fracture and instability

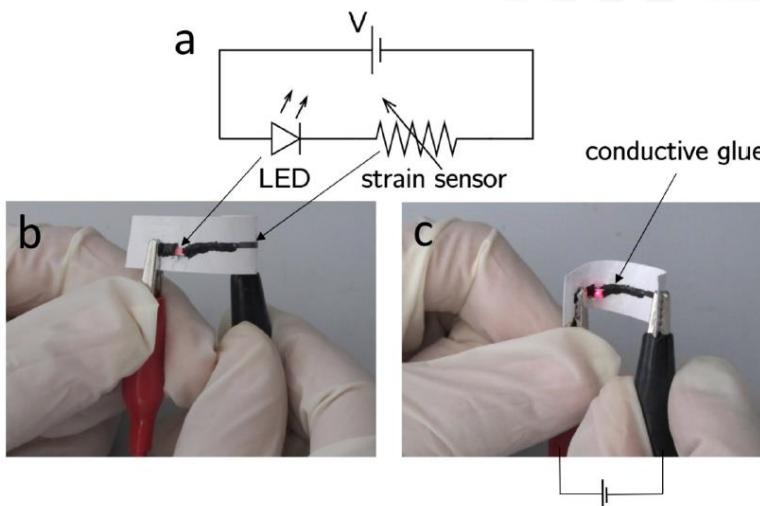


Debonding of stiff coatings from polymeric layers

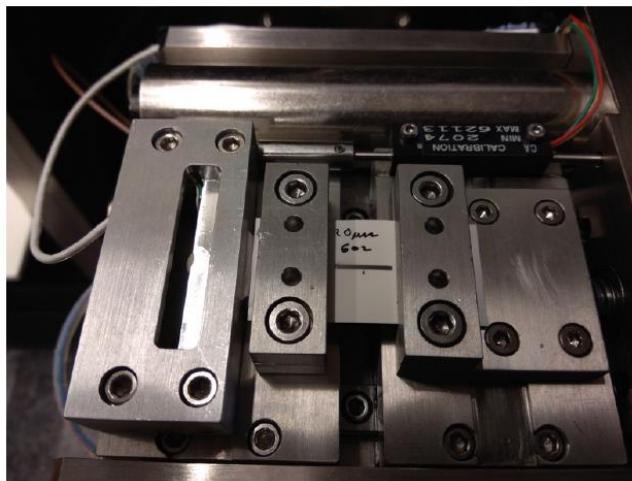


Prediction of
debonding for
flexible electronics
(Silicon on polymer)

Graphene-based electronics inkjet printed on paper



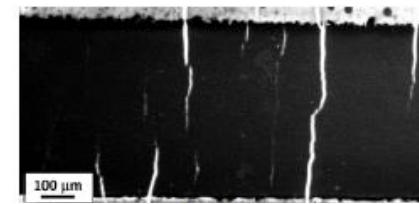
An innovative strain gauge



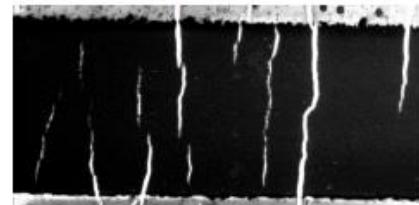
In situ mechanical testing



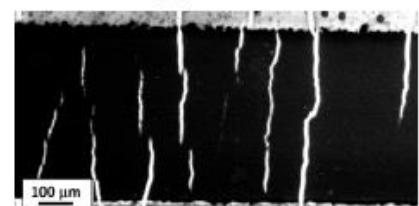
(a) $\varepsilon=0\%$



(b) $\varepsilon=0.4\%$

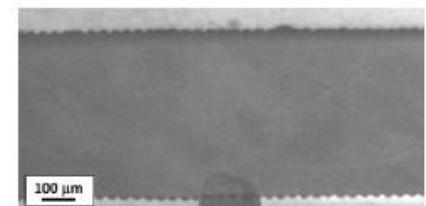


(c) $\varepsilon=0.8\%$

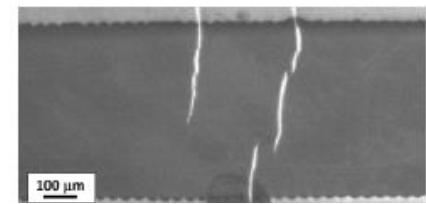


(d) $\varepsilon=1.2\%$

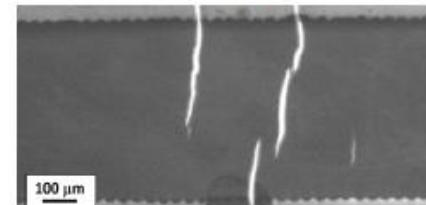
Thick film



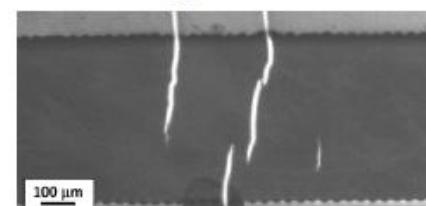
(e) $\varepsilon=0\%$



(f) $\varepsilon=0.4\%$



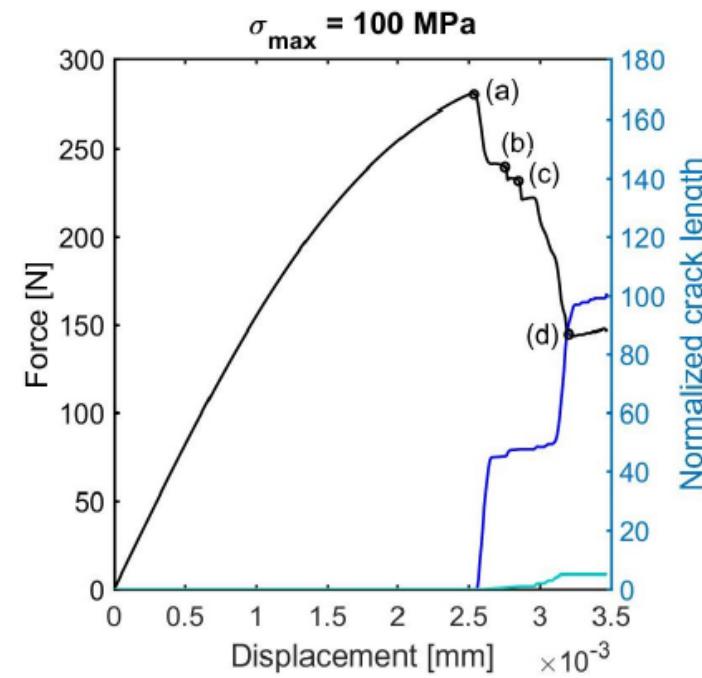
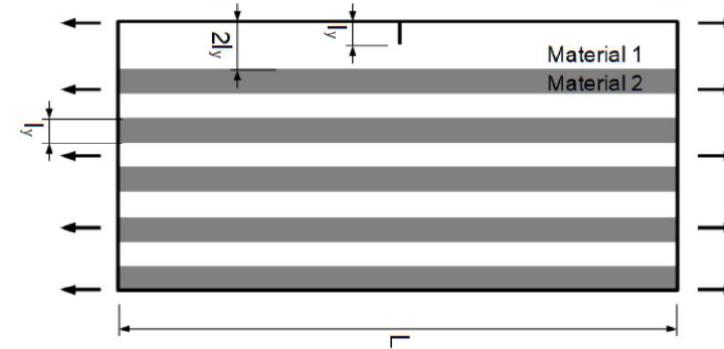
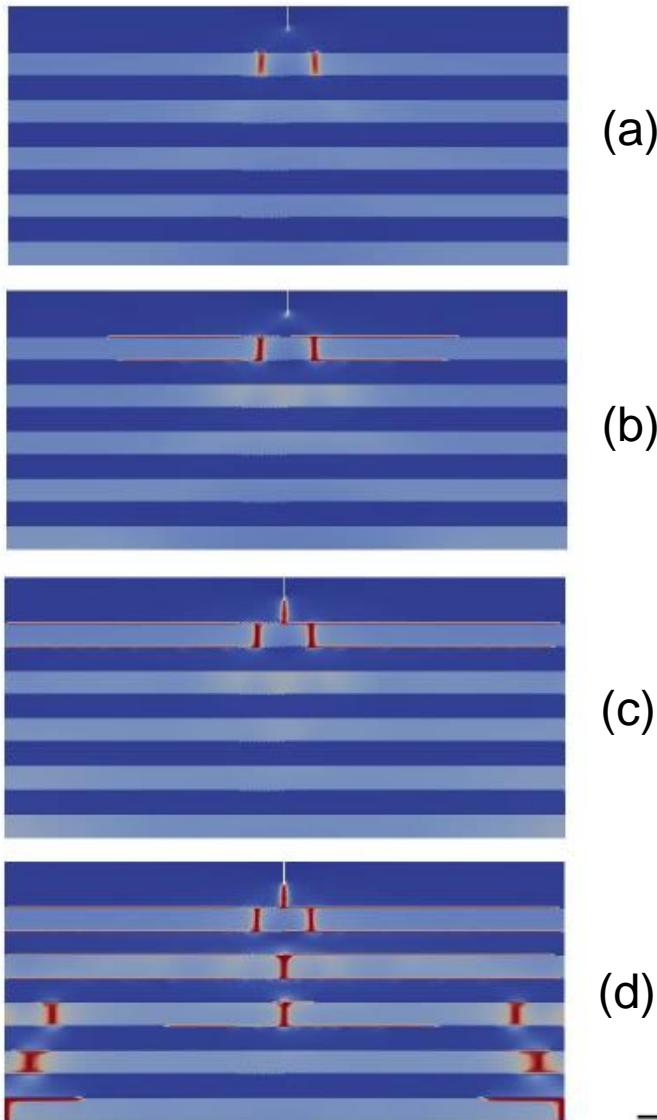
(g) $\varepsilon=0.8\%$



(h) $\varepsilon=1.2\%$

Thin film

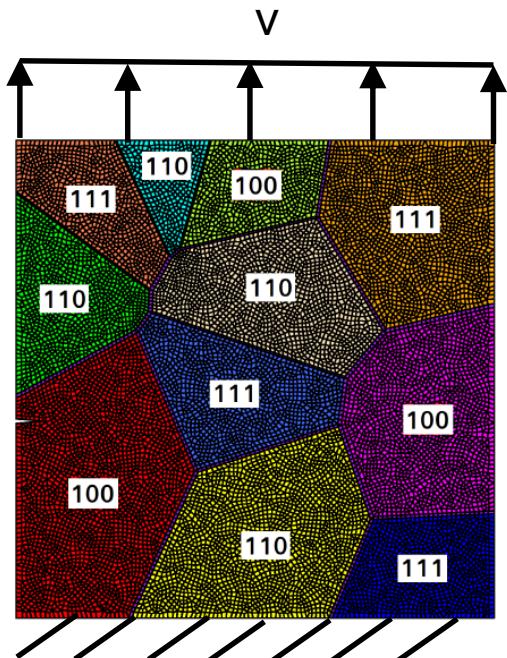
Computational fracture mechanics for laminates



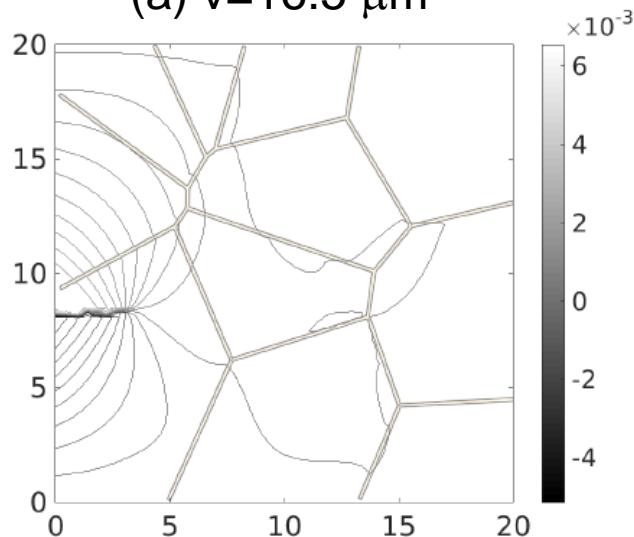
— Force-displacement curve — Delamination + crack propagation — Crack propagation

Computational fracture mechanics of polycrystalline Silicon

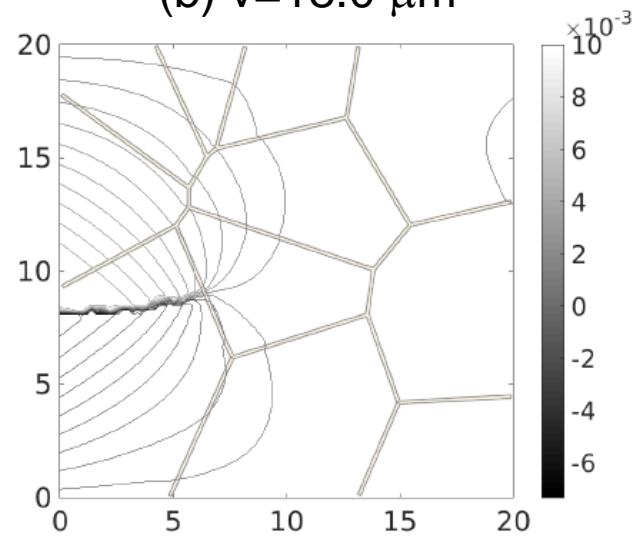
Imposed displacement



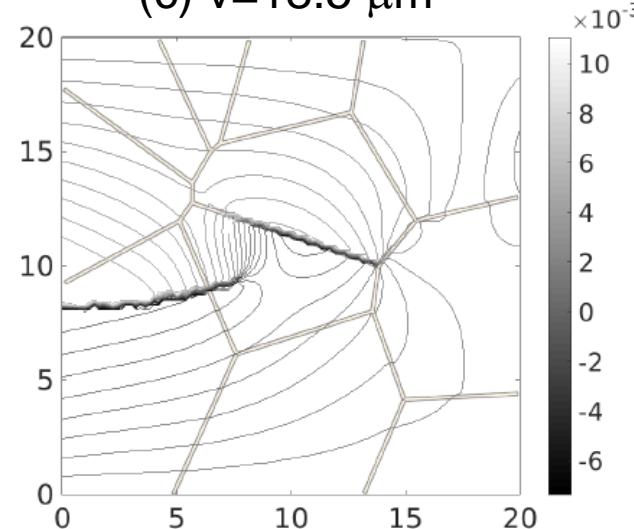
(a) $v=16.5 \mu\text{m}$



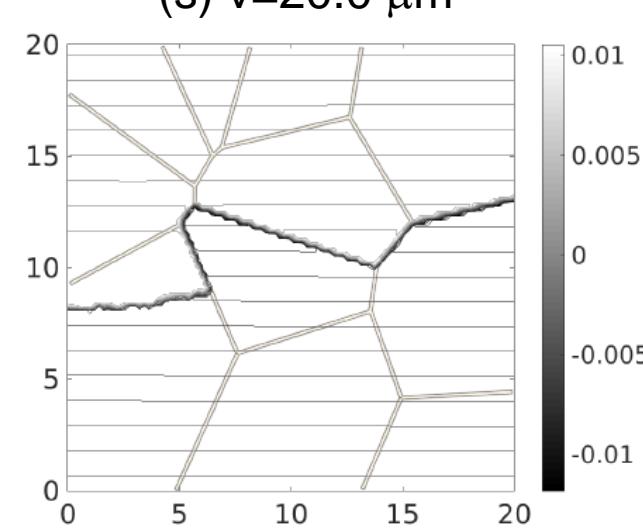
(b) $v=18.0 \mu\text{m}$



(c) $v=18.5 \mu\text{m}$



(d) $v=20.0 \mu\text{m}$



Durability of photovoltaic modules: open issues

Some failure modes of PV modules:

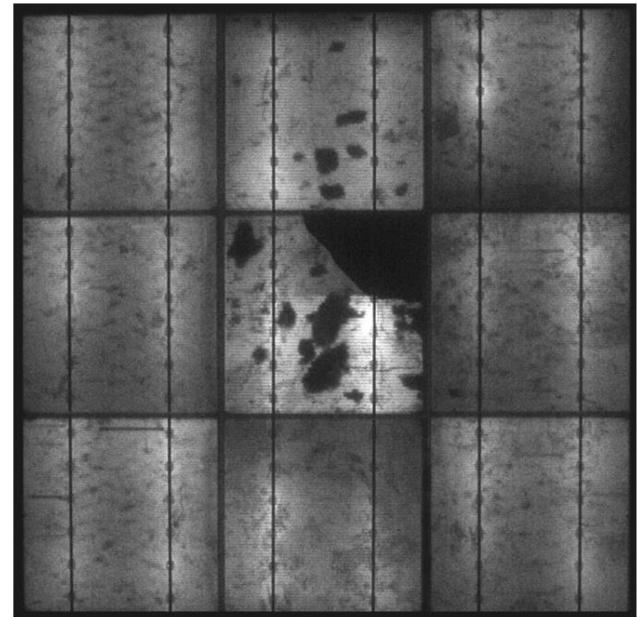
1. Cracks due to mechanical loads
2. Decohesion of the encapsulant
3. Moisture-induced degradation



1



2



3

Durability of photovoltaic modules: multiscale problem

Time scale

Moisture diffusion

20 yrs

PV module

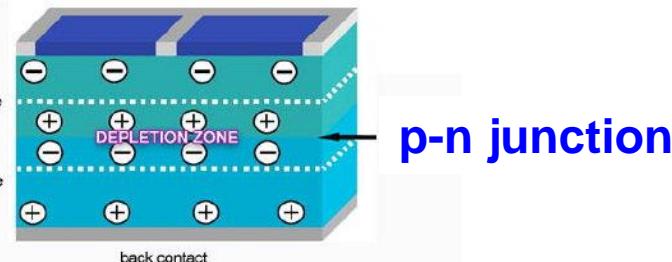
Temperature cycles

1 day

Brittle fracture

1 ms

Silicon solar cell



Recombination effects

1 μ s

10⁻⁴ m

10⁻⁶ m

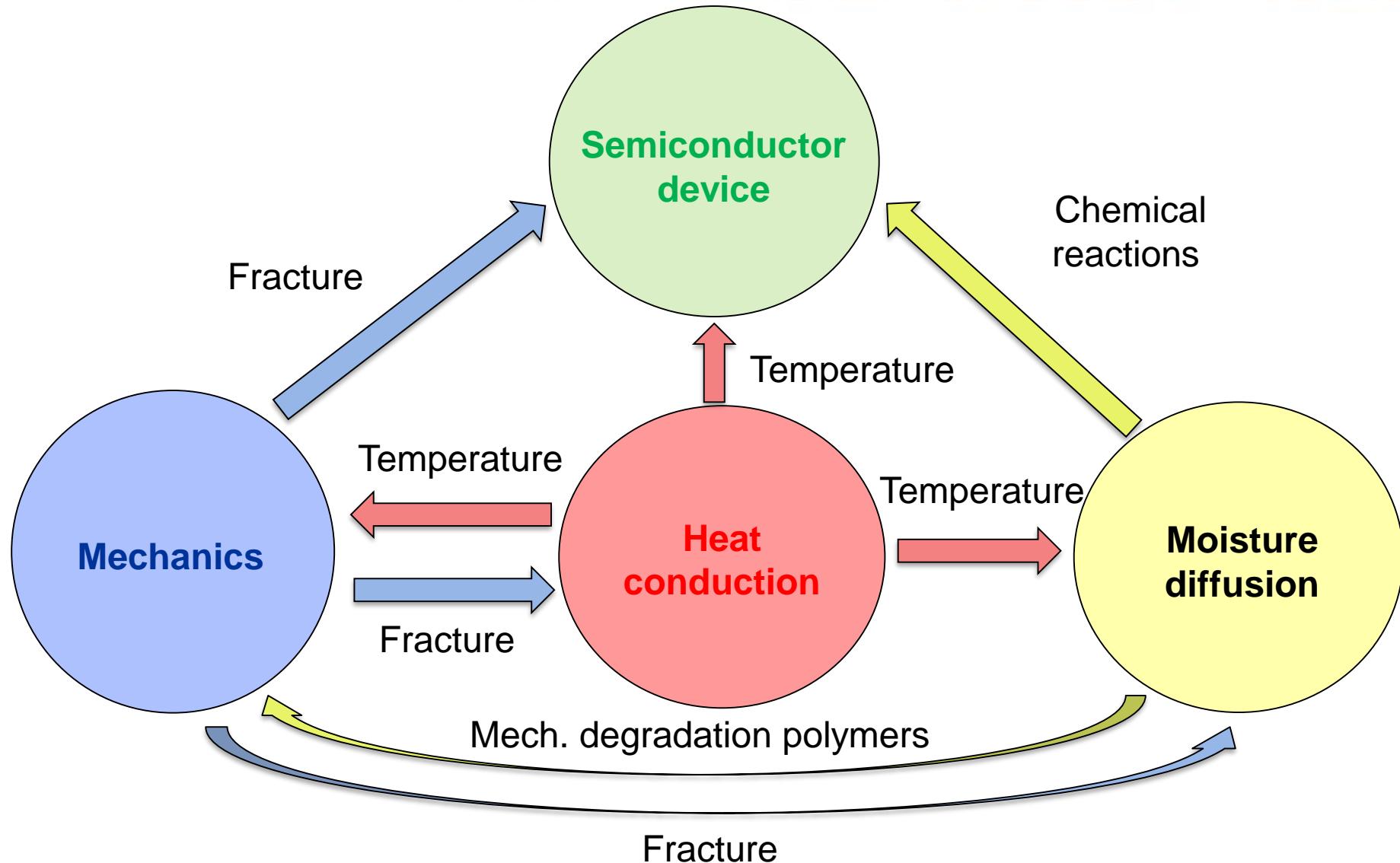
10⁻¹ m

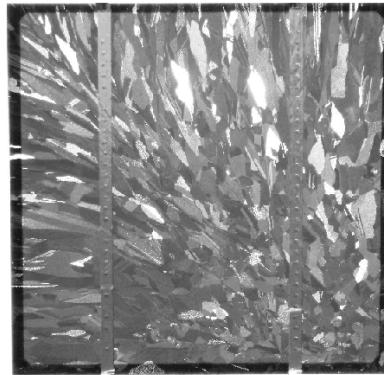
1 m

Length scale



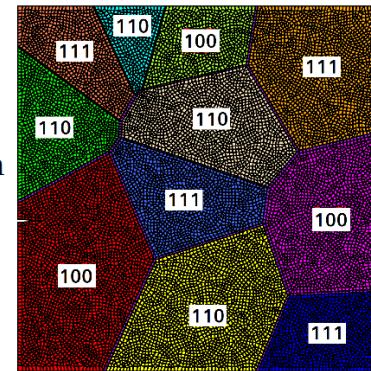
Durability of photovoltaic modules: coupled problem



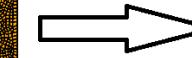


Real polycrystalline
Silicon microstructure

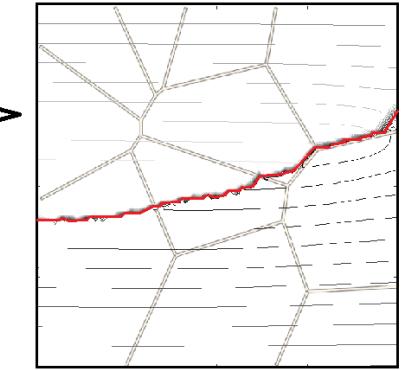
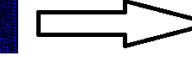
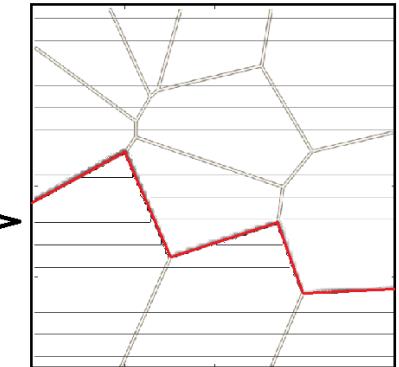
Identification
of grain orientation
distribution



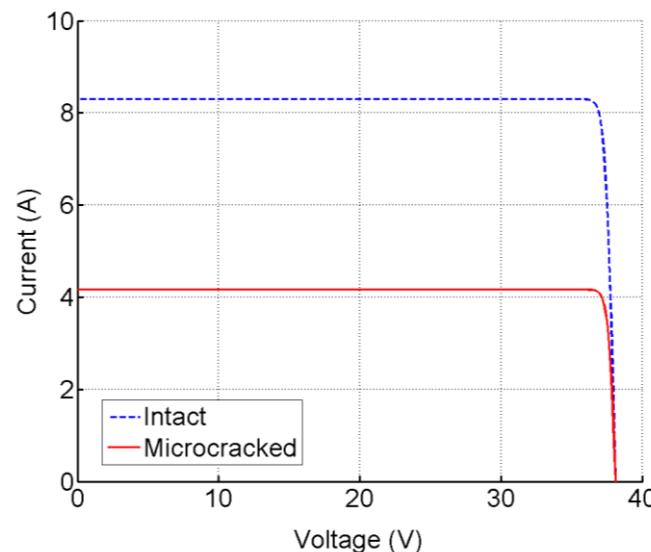
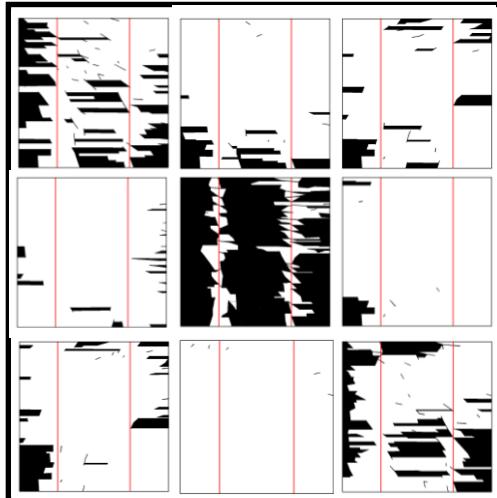
Finite element model



Intergranular fracture

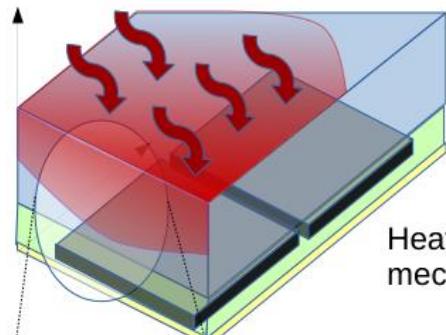


Transgranular fracture

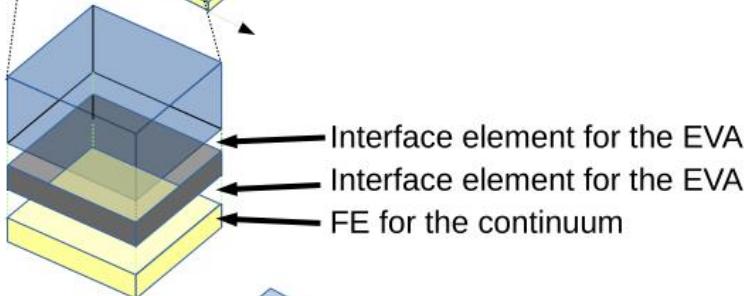


**Prediction of complex
crack patterns,
electrically inactive
areas, power losses**

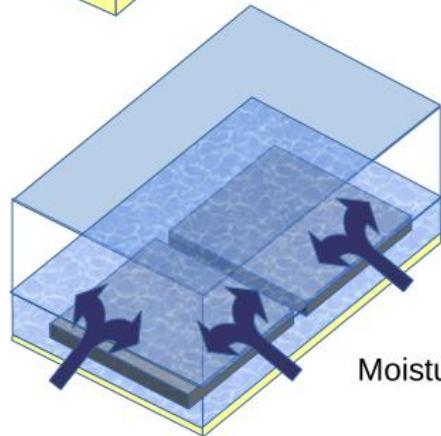
Coupled hygro-thermo-mechanical problems



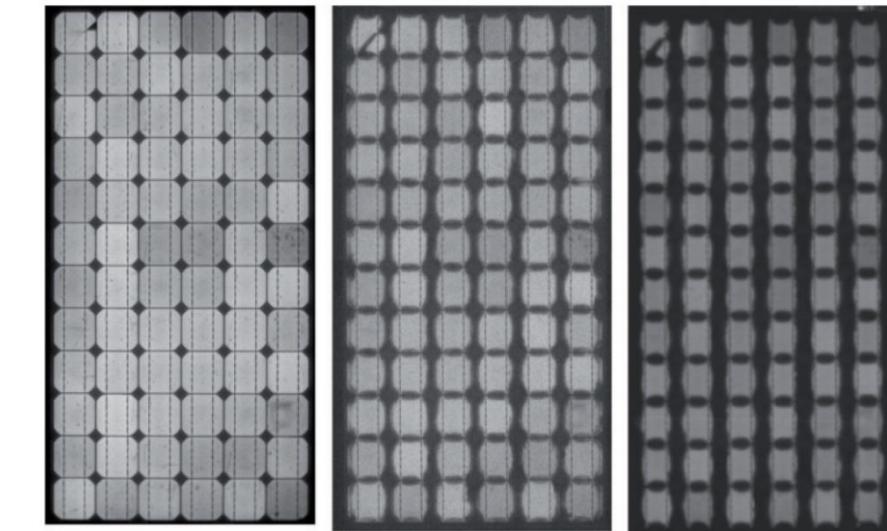
Heat conduction and mechanical loading (3D)



Interface element for the EVA
Interface element for the EVA
FE for the continuum



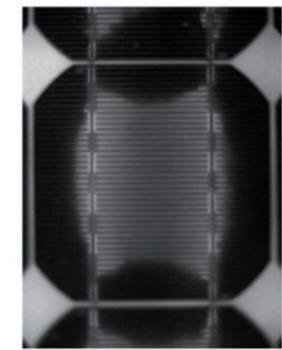
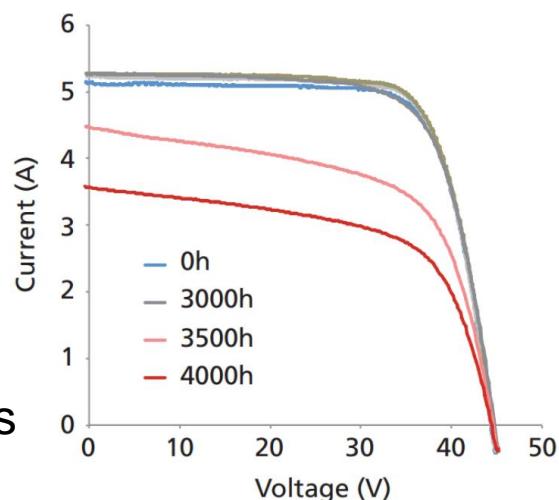
Moisture diffusion (2D)



3000h

3500h

4000h of DH8585

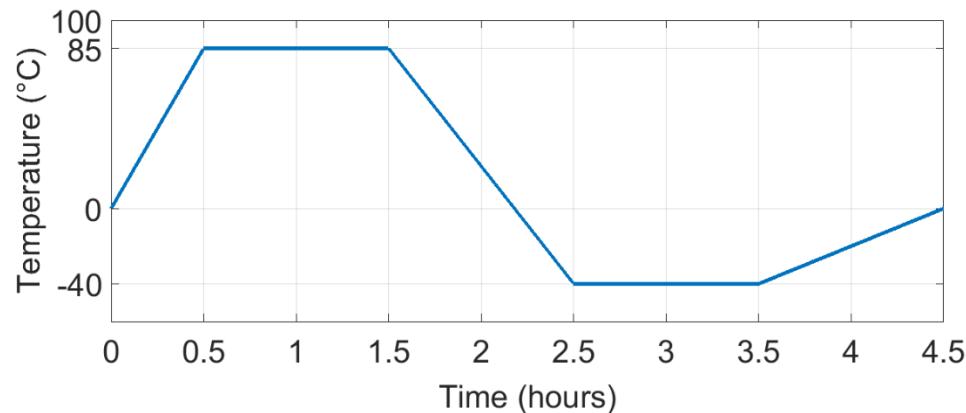


4000h (zoom)

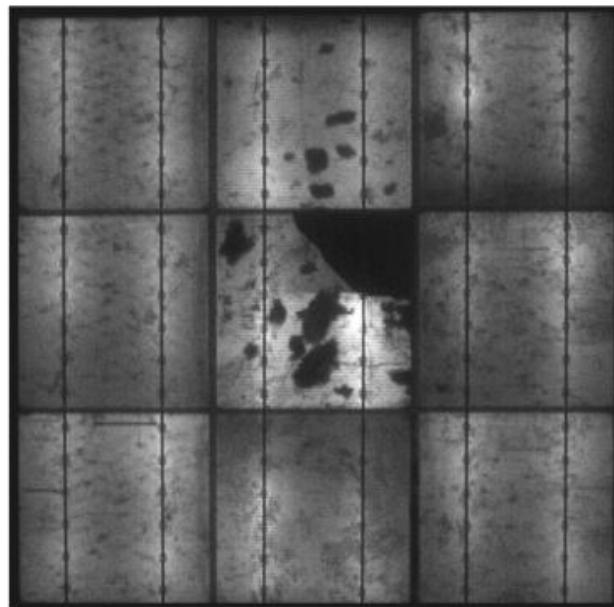
Key features:

- Staggered vs. monolithic FE schemes
- Novel time stepping techniques

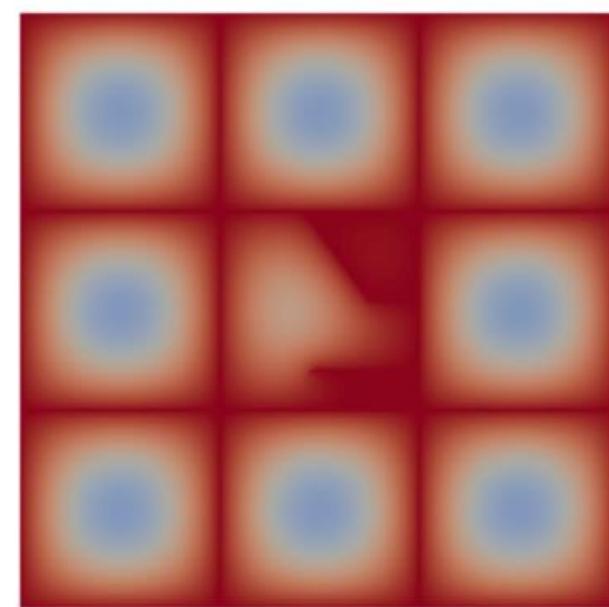
Coupled hygro-thermo-mechanical problems



400 cycles

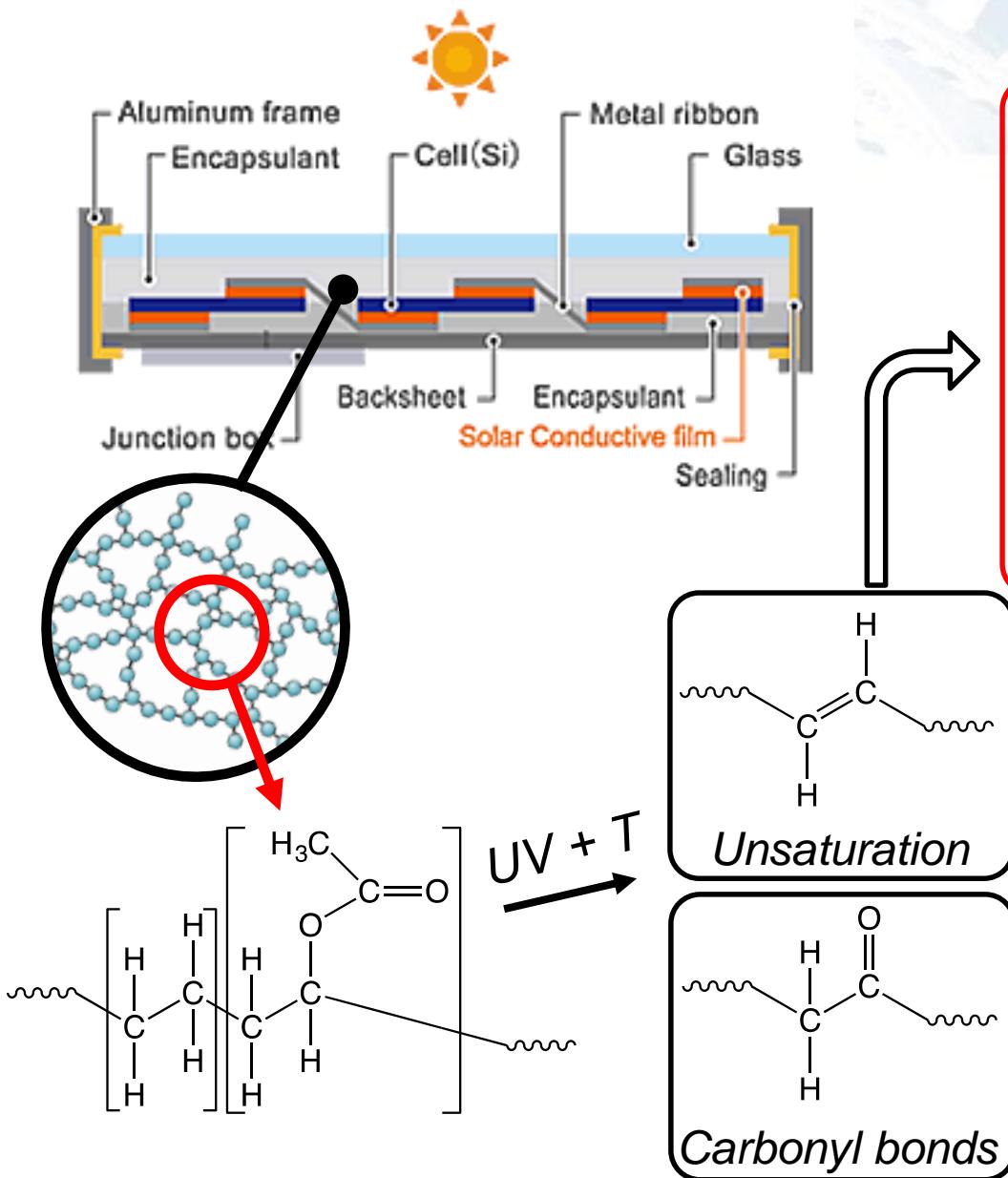


(a) EL image

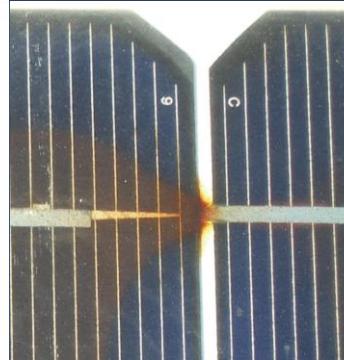


(b) Moisture concentration

Chemical degradation



Acetic acid (CH_3COOH):

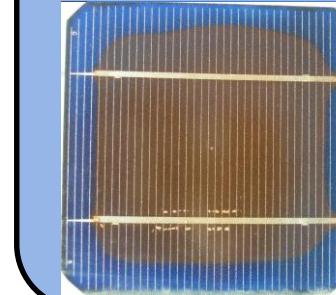


Ag corrosion



Snail trails

Browning

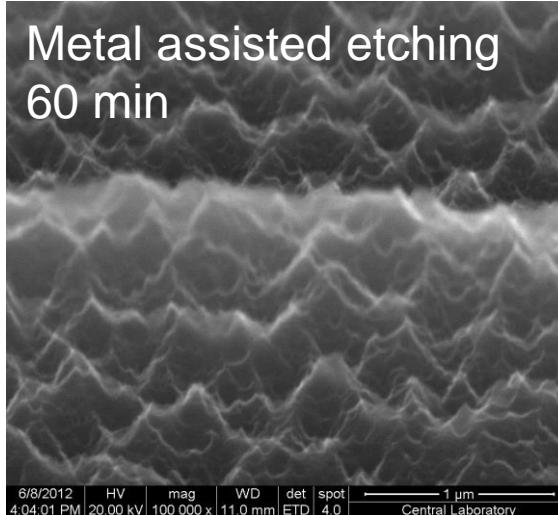


Moisture sorption + gas formation + overheating

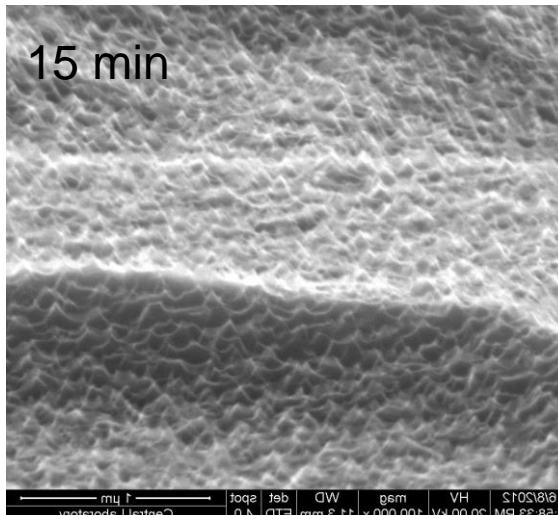


Surface texturing of Silicon

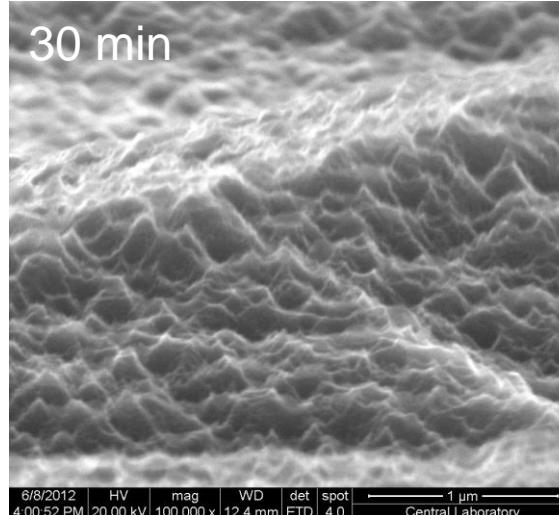
Metal assisted etching
60 min



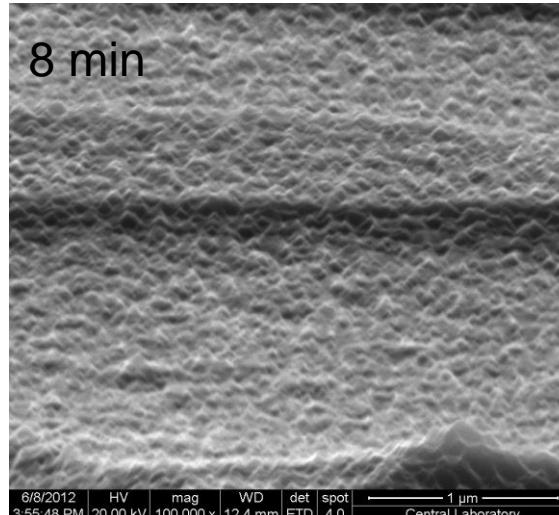
15 min



30 min



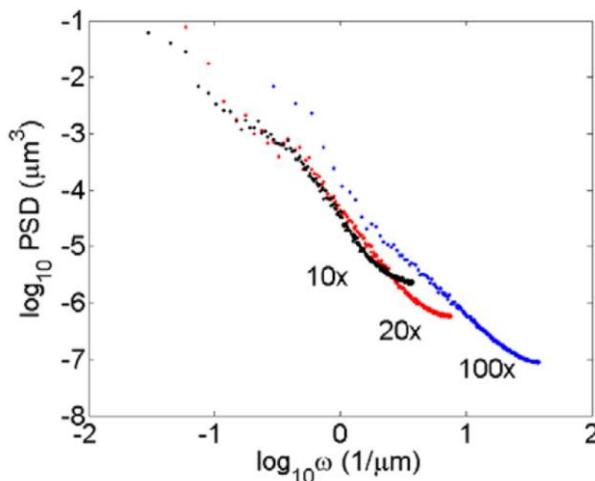
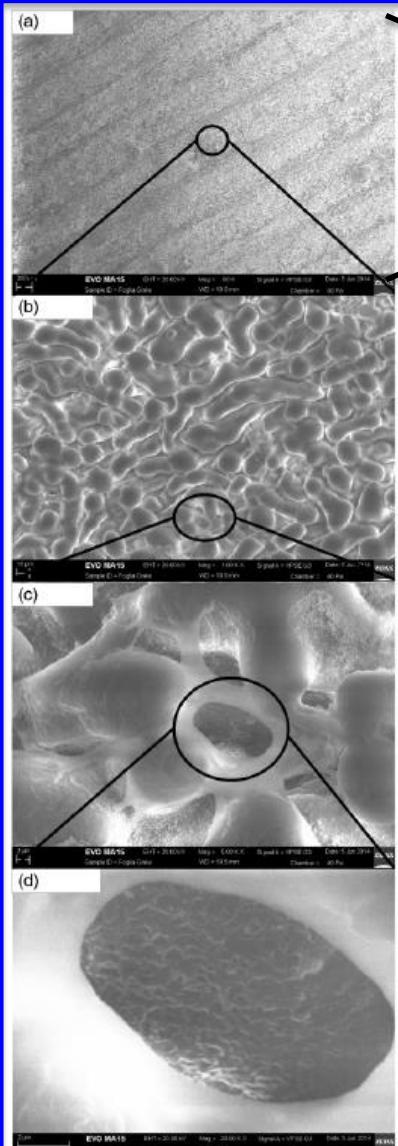
8 min



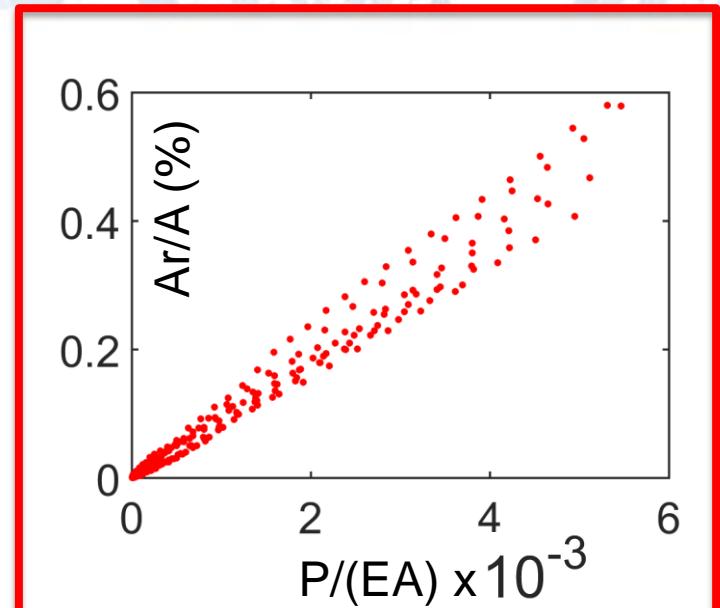
Key features:

- The effect of roughness on leakage
- Light reflectance
- Thermal and electric resistance of the interface
- Wettability
- Adhesion

Multiscale analysis of surface texturing



Multi-scale roughness characterization

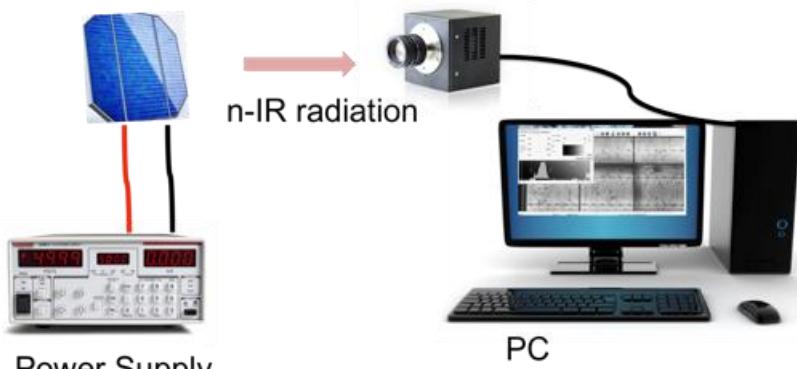


Contact mechanics simulation (BEM)

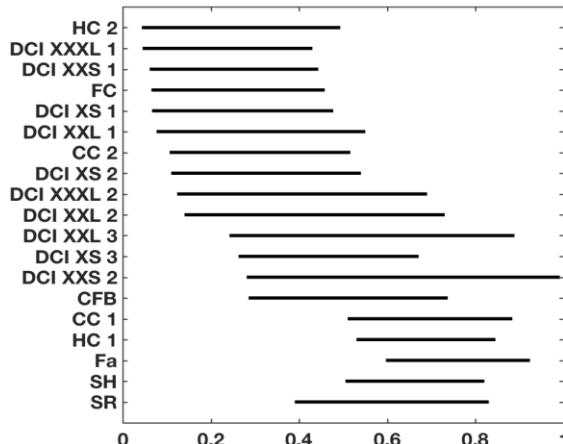
- Normal contact
- Tangential contact
- Wear prediction
- Contact conductance

Electroluminescence (EL)

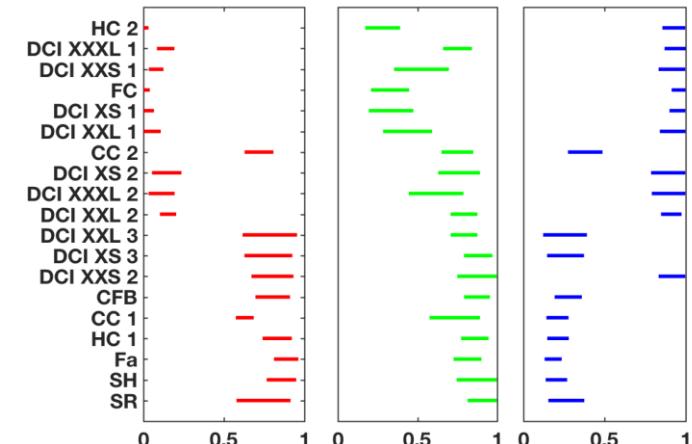
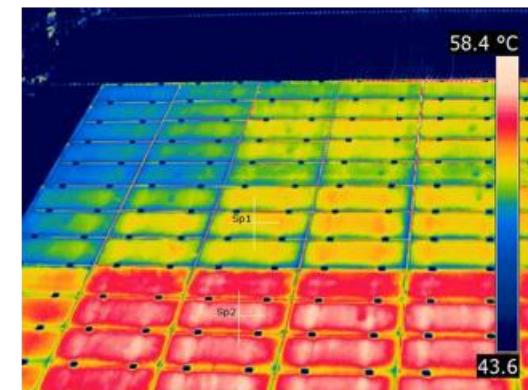
Solar cell Cooled Camera



Power Supply



Thermography (IR)

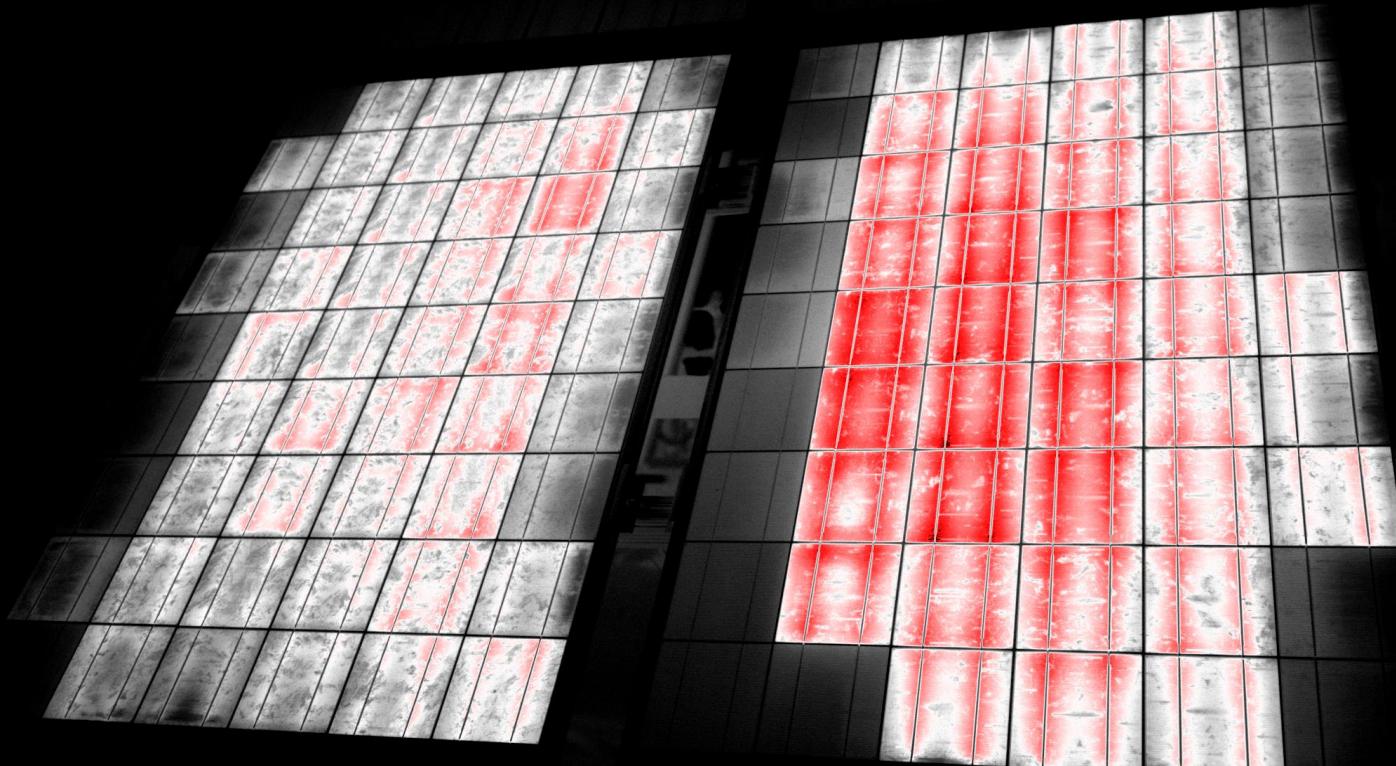


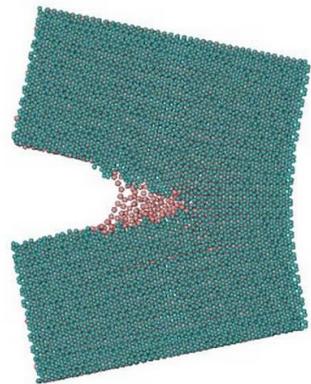
Outreach and collaboration with the International Energy Agency

GUIDELINES FOR EL OUTDOOR QUALIFICATION OF PV SYSTEMS

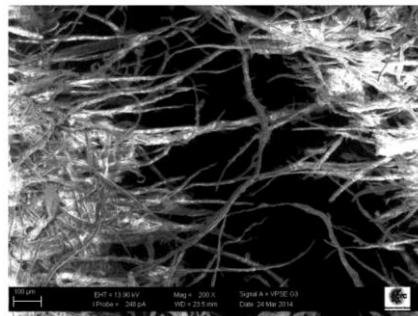
Intersolar Europe Conference, 30 May 2017, Munich, Germany

PV Reliability & Assessment of Technical Risks in PV Investments

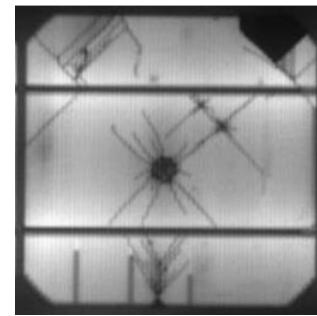




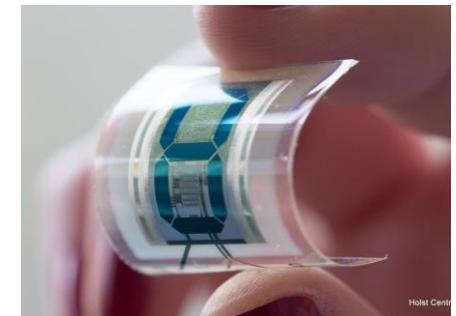
Graphene coatings



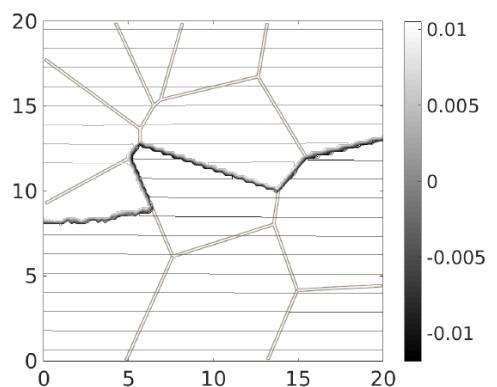
Fibrous materials



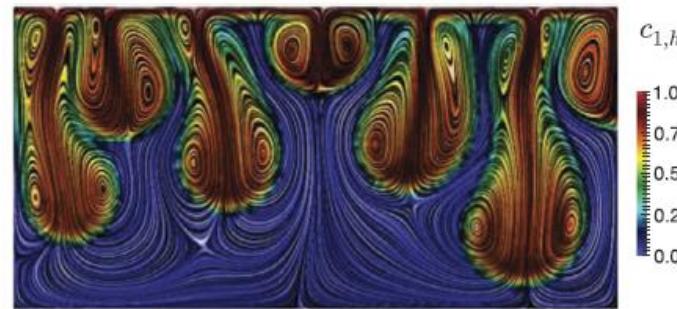
Photovoltaics



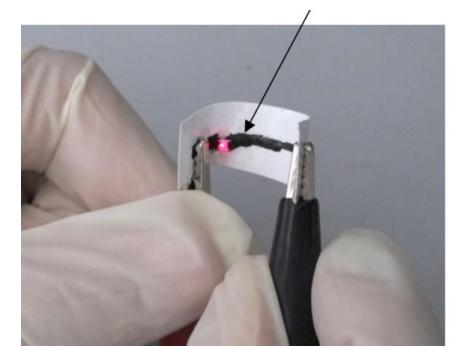
Flexible electronics



Polycrystals



Advection-reaction-diffusion systems



Printable electronics

Collaborations and technology transfer

International Energy Agency
Photovoltaic Power Systems Programme (PVPS)



Joint Research Centre
Institute for Energy and Transport



Institute for Solar Energy Research
Hamelin, Germany



Acknowledgements

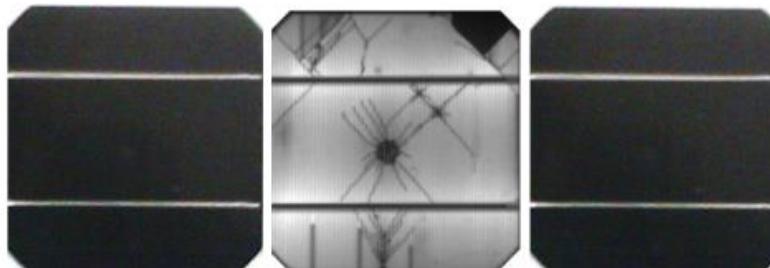


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<https://www.facebook.com/fanpagemusam>

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



European Research Council
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