IMT Institute for Advanced Studies

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Emergent properties in interface mechanical problems:

A paradigm of organized complexity

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Outline

1. Organized complexity & emergent properties in interface problems
2. An example in contact mechanics
3. An example in fracture mechanics
4. A multiphysics application: photovoltaics
5. Ongoing research topics

Acknowledgements

Unterstützt von / Supported by
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Emergent properties in ordered complexity

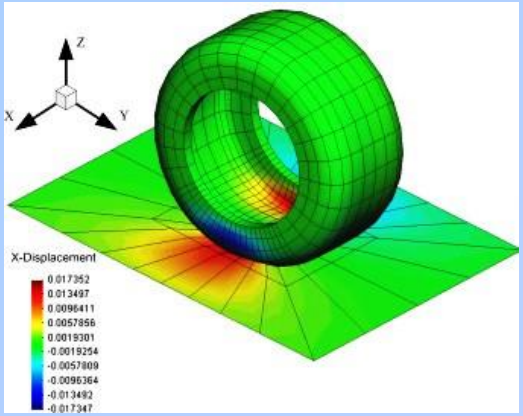
Classical examples of complex systems:

- **Earthquakes**
- **Climate systems**
- **Living systems**
- **Social systems**
- **Economical systems**

Organized complexity resides in the non-random, or correlated, nonlinear interaction between the parts of a system

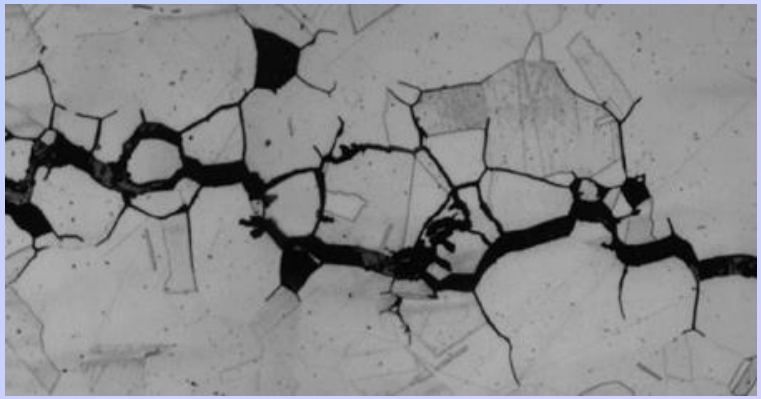
Coordinated systems exhibit emergent properties not easily predictable from the properties of their constituents

Organized complexity in interface problems



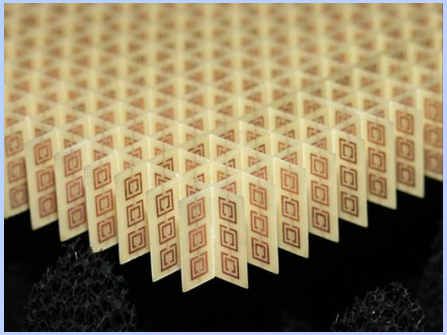
Contact mechanics

- Scaling of contact properties (friction coefficient, adhesion, thermal contact conductance)



Fracture mechanics & fatigue

- Scaling of strength and toughness



Metamaterials

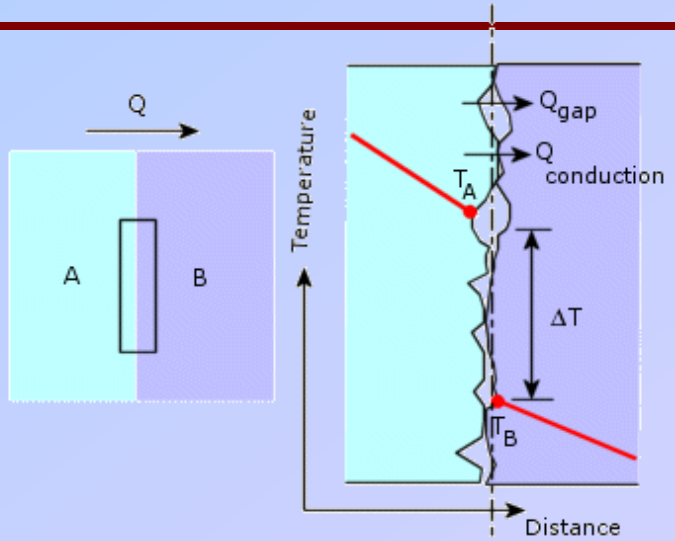
- Scaling of optical and elecromagnetic properties

Common features:

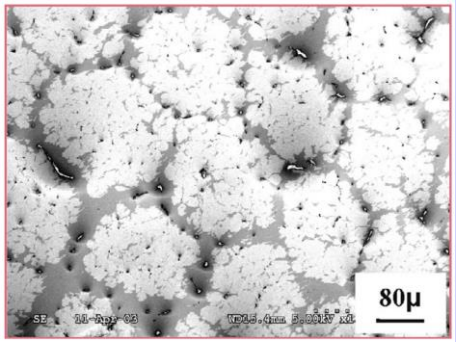
Nonlinear relations; multiple scales; fractality / hierarchy

Two examples of emergent properties

(1) Interface thermal resistance due to roughness



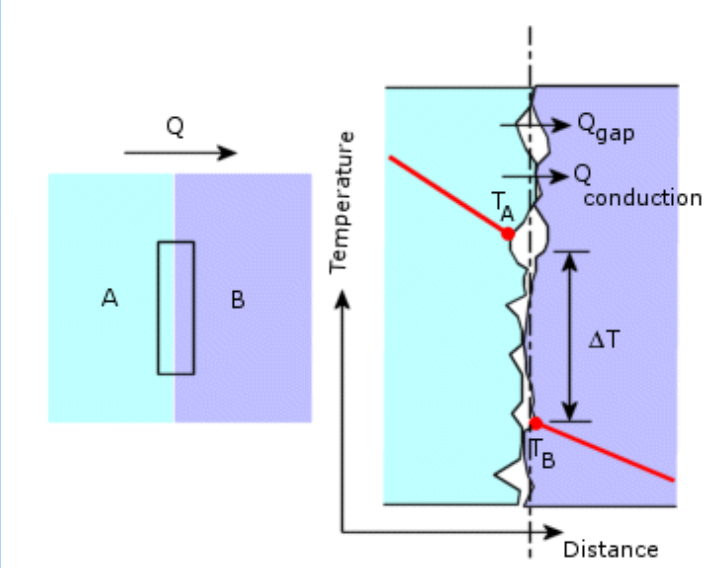
(2) Flaw-tolerance of hierarchical polycrystalline materials

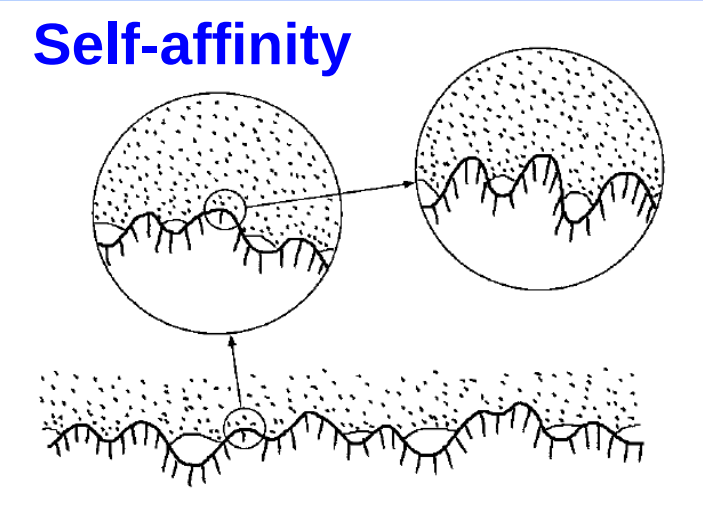


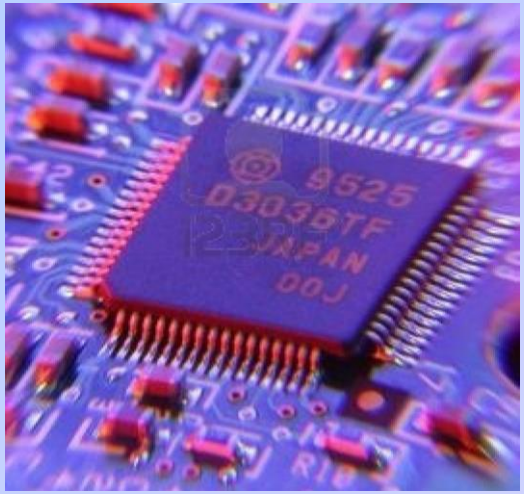
Aim: **study of the emergence of macro-properties from micro-properties (bottom-up approach)**

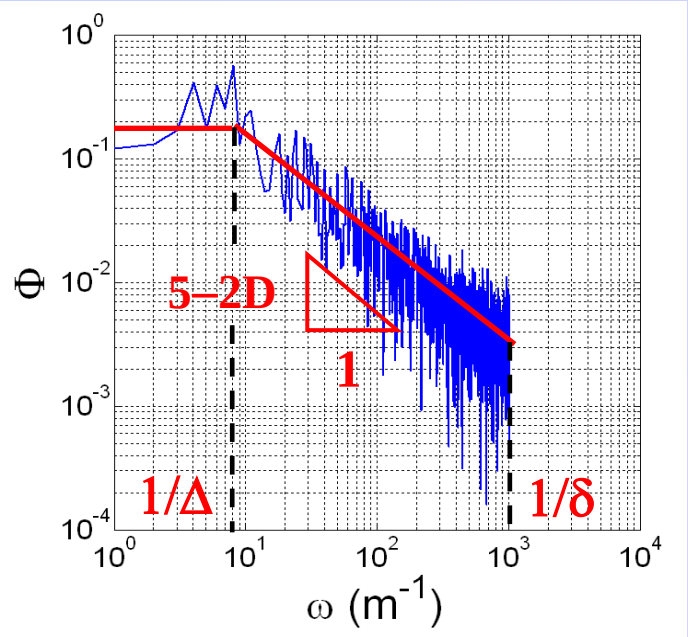
Methods: **nonlinear mechanics, computational methods, optimization**

Interface contact conductance





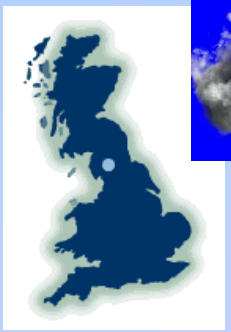


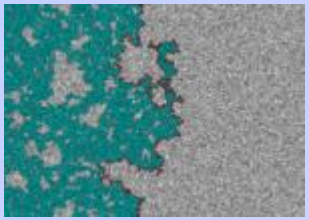


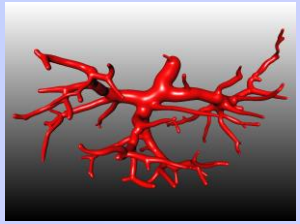
Fractality

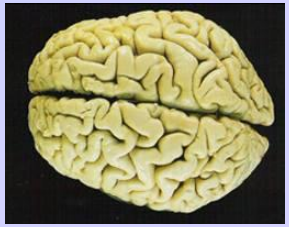
- **Self-affinity (even of a random nature)**
- **Non integer dimension**

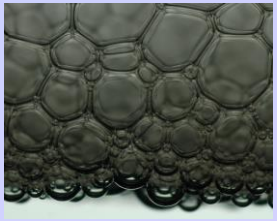
Examples:

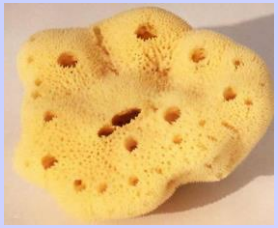












dim. 1÷2

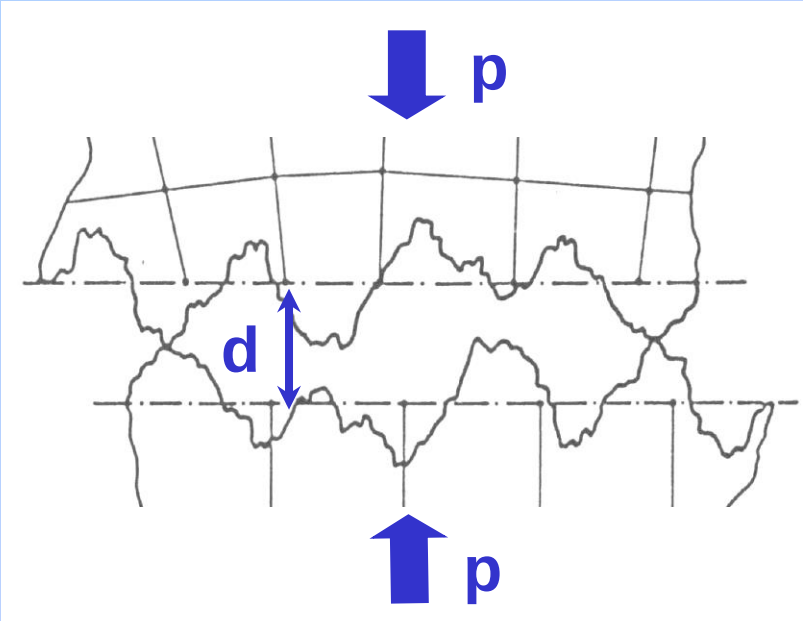
- mountains profiles
- clouds profiles
- coastlines profiles
- river patterns
- diffusion fronts
- moon craters
- arterial systems

dim. 2÷3

- sponge-cloths
- foams
- brain folds
- universe mass

Interface contact conductance

The contact conductance is proportional to the contact stiffness (Barber, PRS 2003; Paggi and Barber, IJHMT 2011):



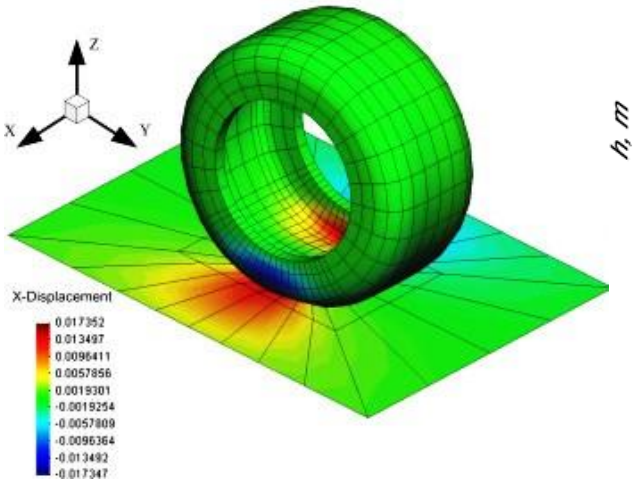
$$C = -\frac{2}{\rho E}\frac{\mathrm{d}p}{\mathrm{d}d}$$

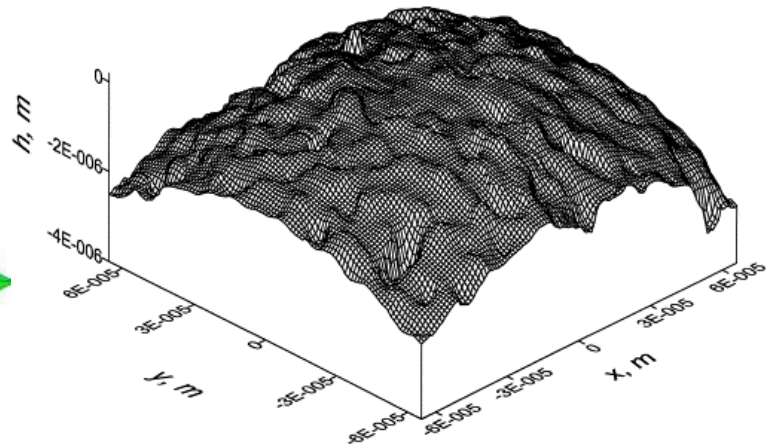
$$\tilde{C} \equiv C\rho\Delta \qquad \tilde{d} = \frac{d}{\sqrt{m_0}} \qquad \tilde{p} = \frac{p\Delta}{E\sqrt{m_0}}$$

$$\tilde{C} = \tilde{p}^{\beta}\,\Phi_2\left(\frac{\delta}{\Delta}, \frac{L}{\Delta}, D\right) \qquad \tilde{p} = A\left(\tilde{d}_0 - \tilde{d}\right)^{\frac{1}{1-\beta}}$$

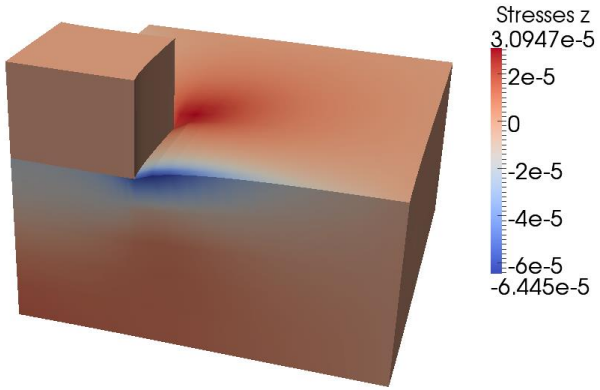
Inverse problem

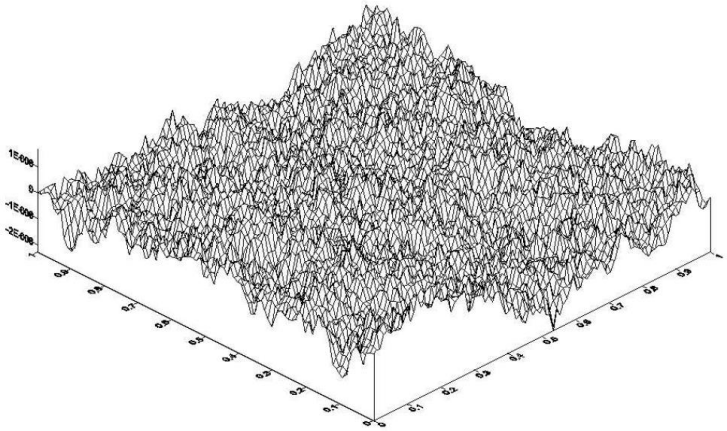
Problem: extract the interface contact conductance (nonlinear mesoscopic property) from global stiffness data (emergent macroscopic property)





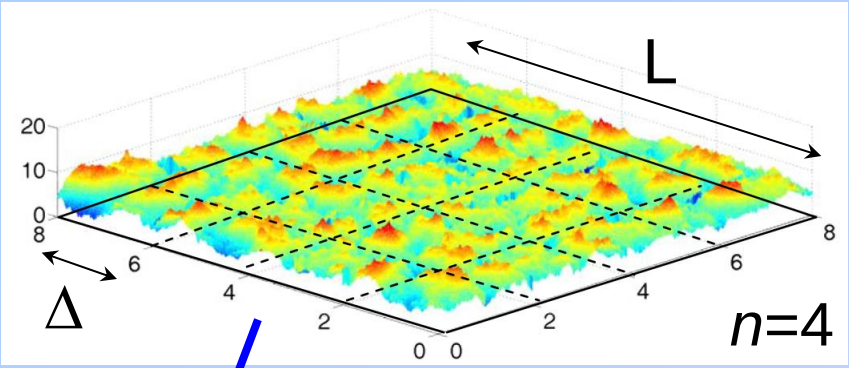
Macroscopic curvature effects



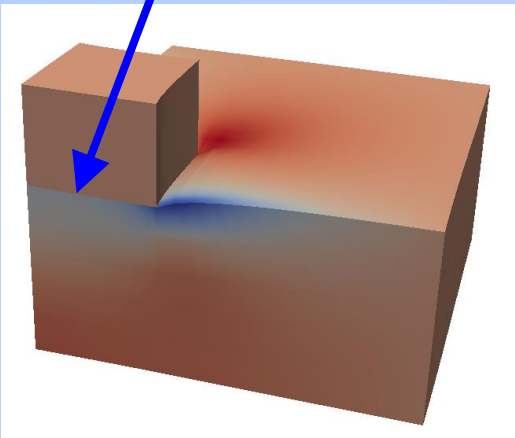


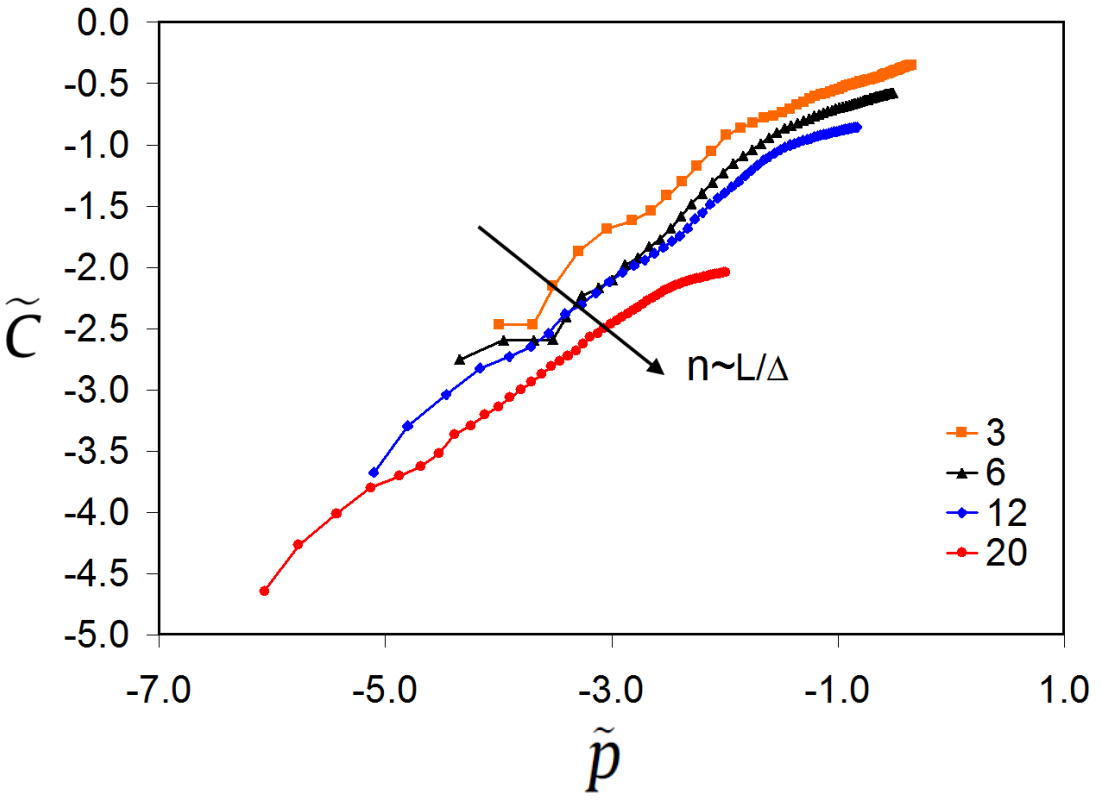
Finite size effects (boundary effects)

Global stiffness by varying the punch size L

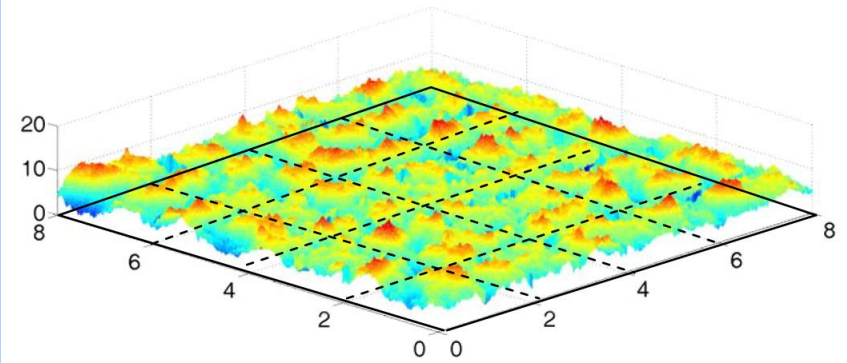


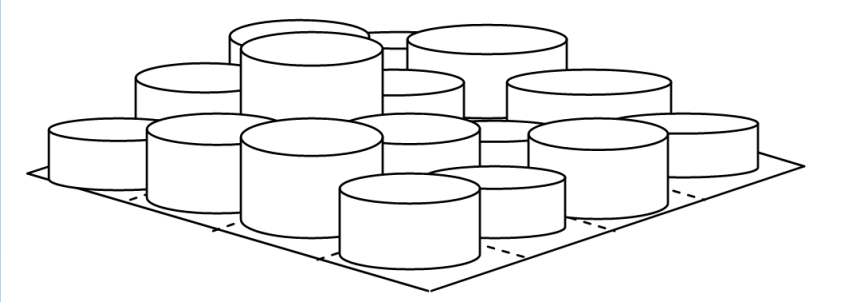
Rough punch composed of *n* x *n* RMD patches

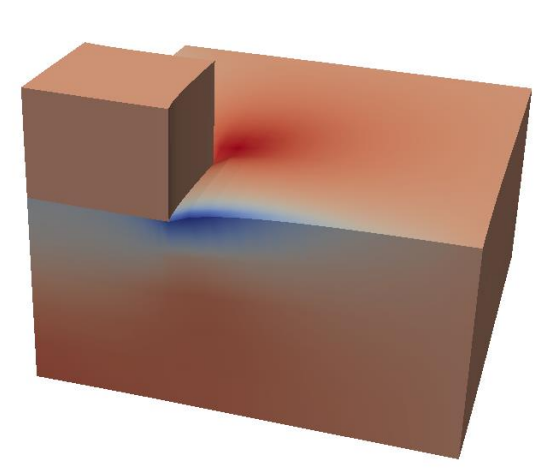




Proposed solution strategy







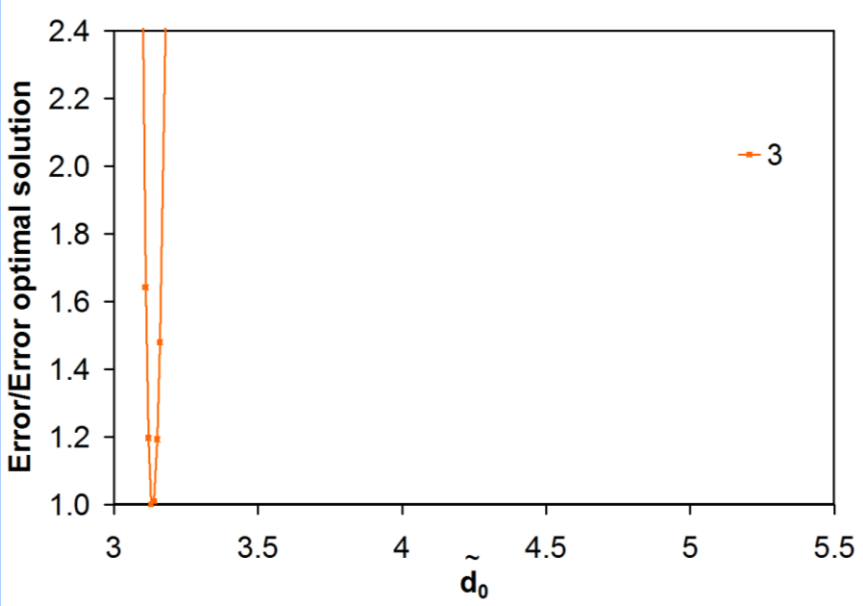
1. Solve the contact problem between the rough punch and the half-plane (global solution)

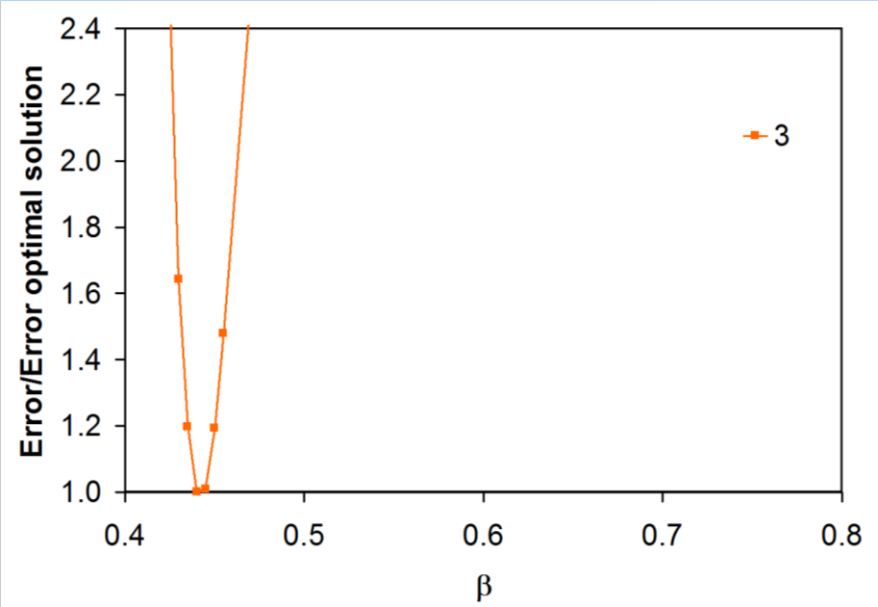
2. Imagine the surface as a collection of nonlinear punches whose constitutive equation is:

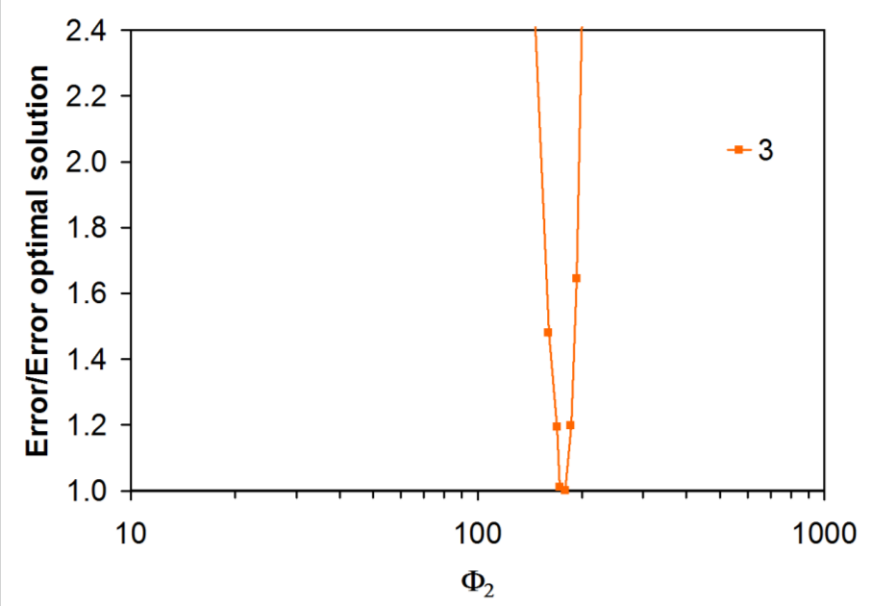
$$\tilde{p} = A\left(\tilde{d}_0 - \tilde{d}\right)^{\frac{1}{1-\beta}}$$

3. Solve the contact problem and find the optimal values of the 3 free parameters to match the global solution

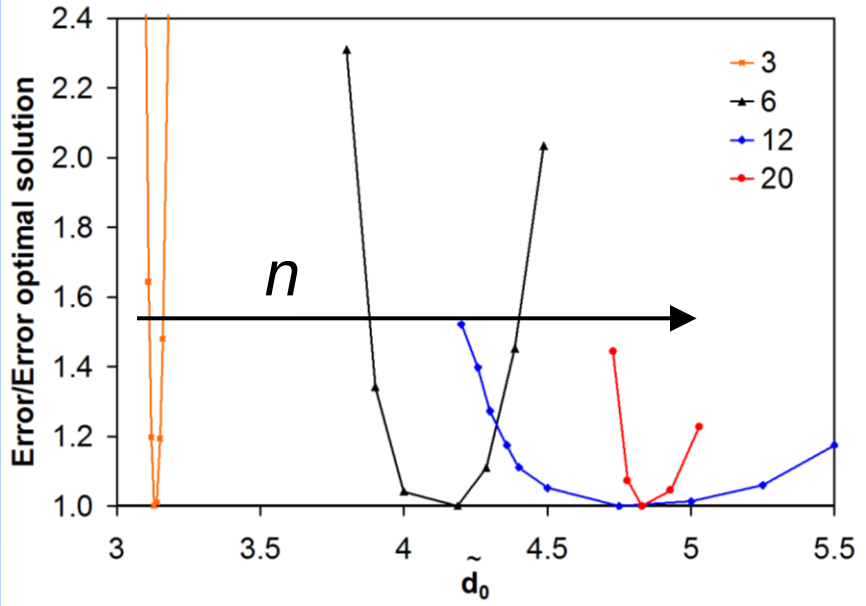
Result of the optimization problem

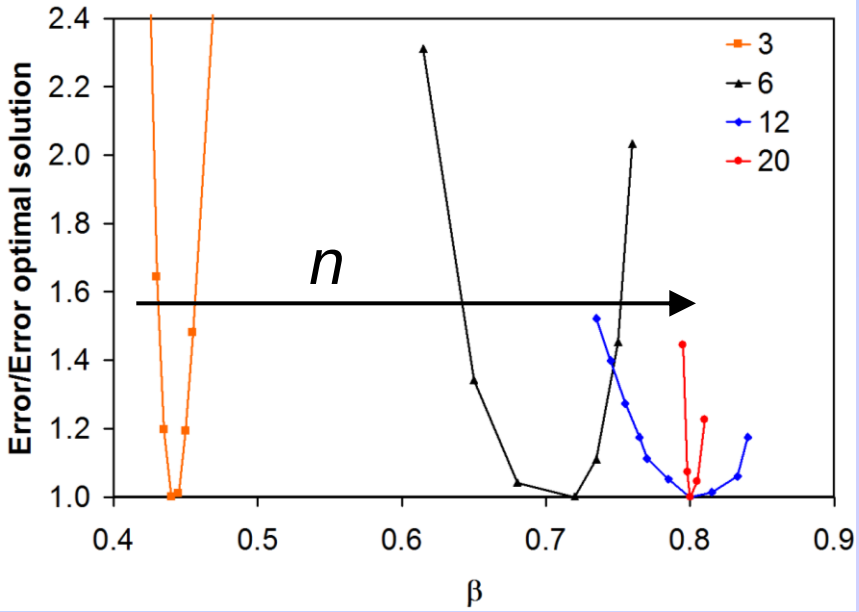






Result of the optimization problem



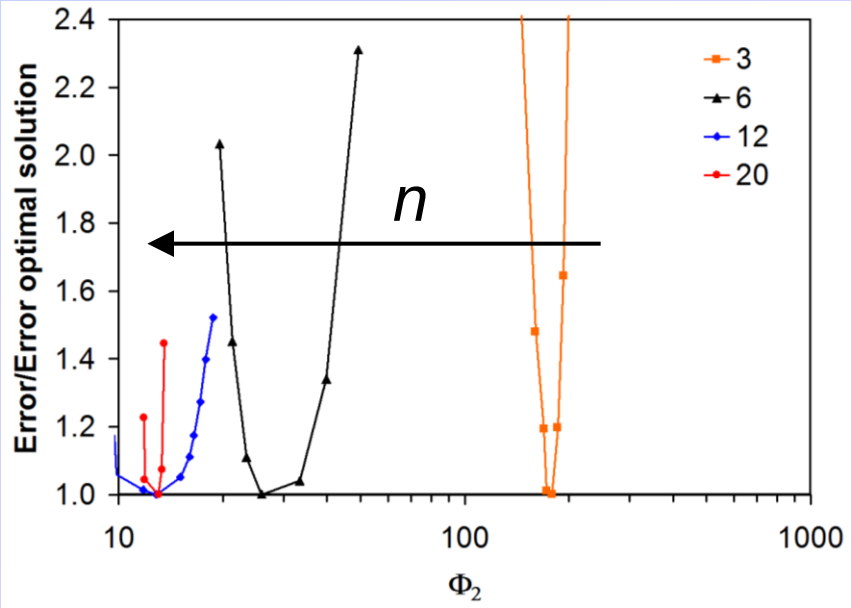


Optimal solution independent of BCs (model-independent interface contact conductance):

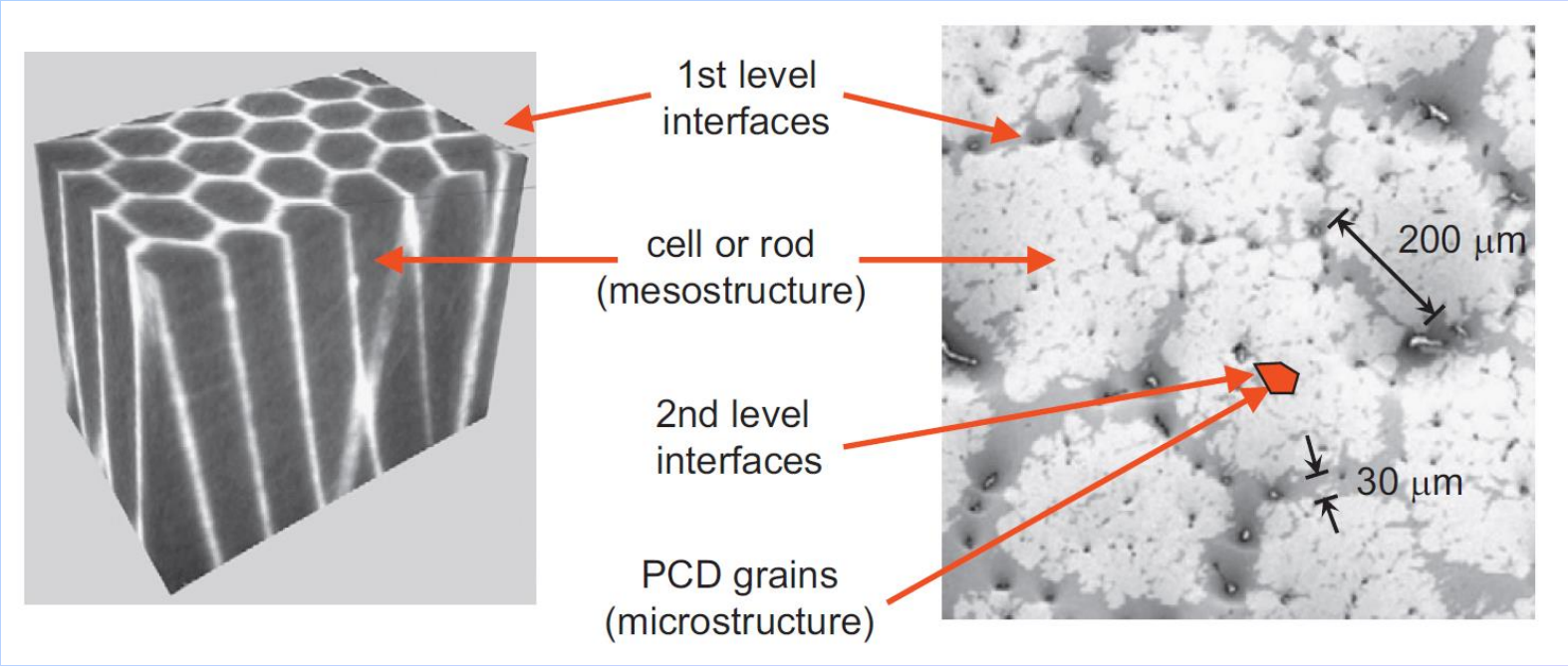
$\tilde{d}_0$=4.83
β=0.80
Φ_2=13

$$\tilde{C} = 13\tilde{p}^{0.8}$$

$$\tilde{p} = 0.01\left(4.83 - \tilde{d}\right)^5$$



Hierarchical polycrystalline materials

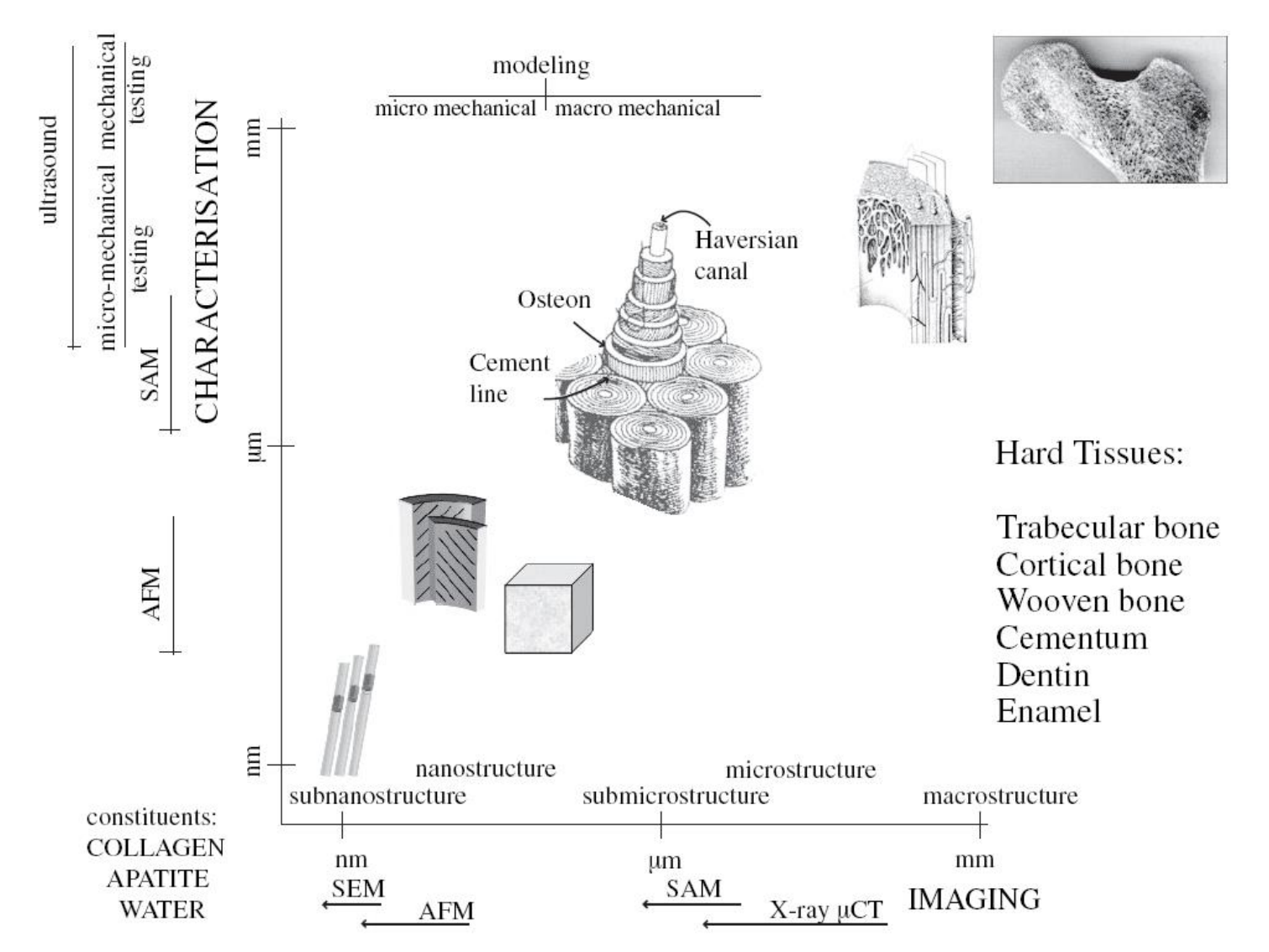


How do the strength depend on the interaction between interfaces at different scales?

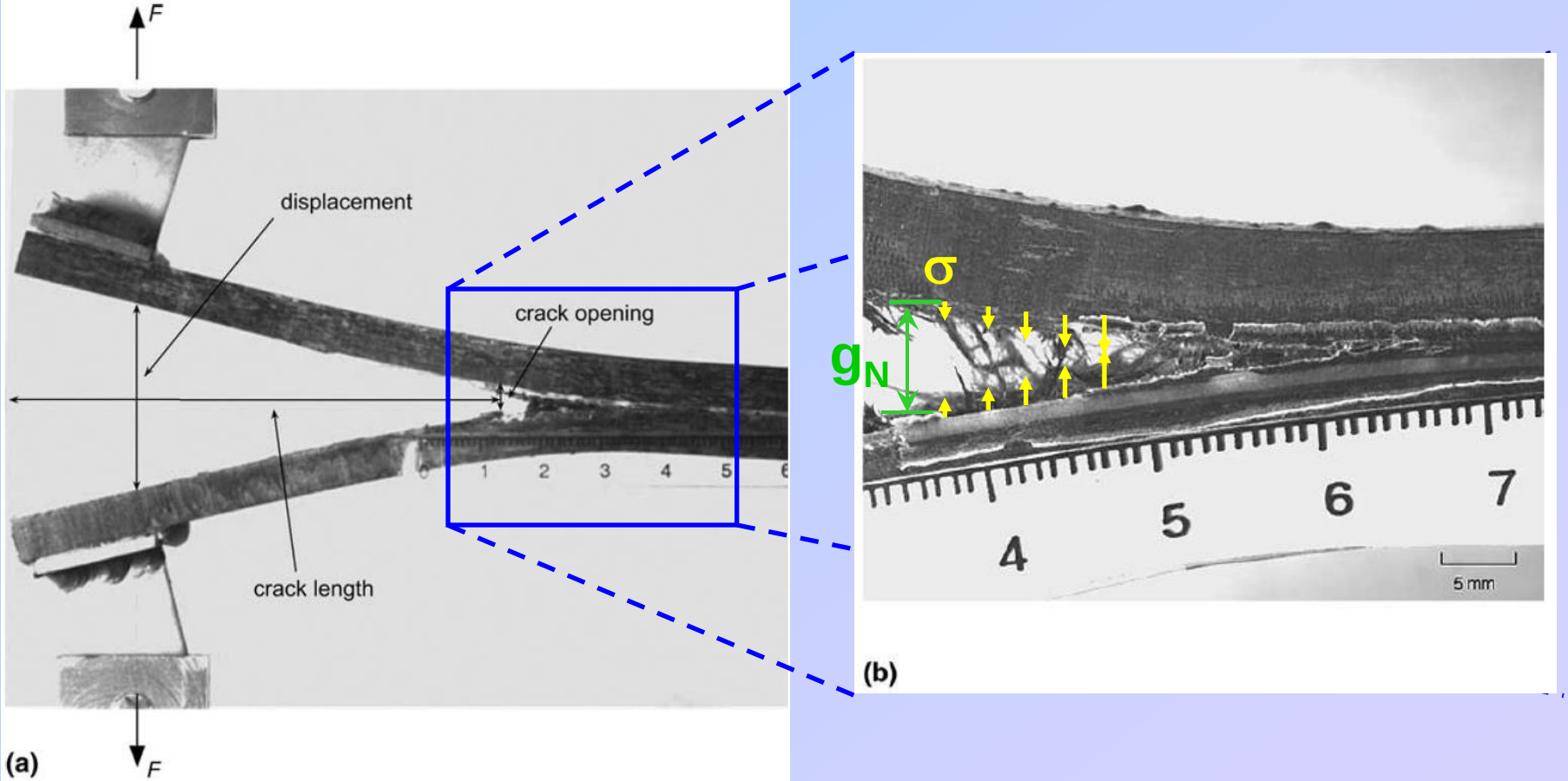
Is there any emergence of an optimal configuration to tolerate defects (flaw tolerance)?

M. Paggi, P. Wriggers (2012) ***J. Mech. Phys. Solids***, 60:557-571.

Mimicking nature: interfaces at different scales

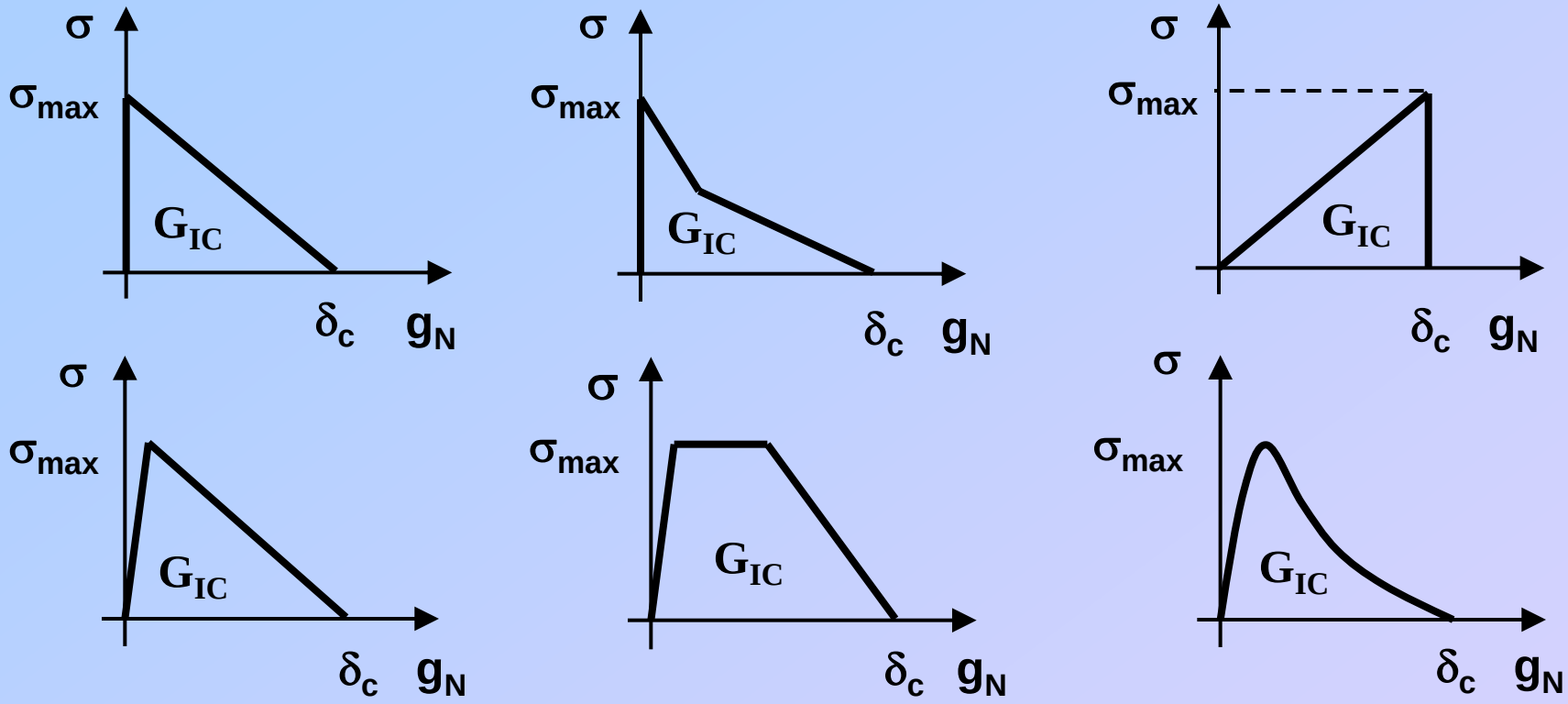


The Cohesive Zone Model



S. Li, M.D. Thouless, A.M. Waas, J.A. Schroeder, P.D. Zavattieri (2005) **Composites Science and Technology** 65:281-293.

The Cohesive Zone Model



Open issues:

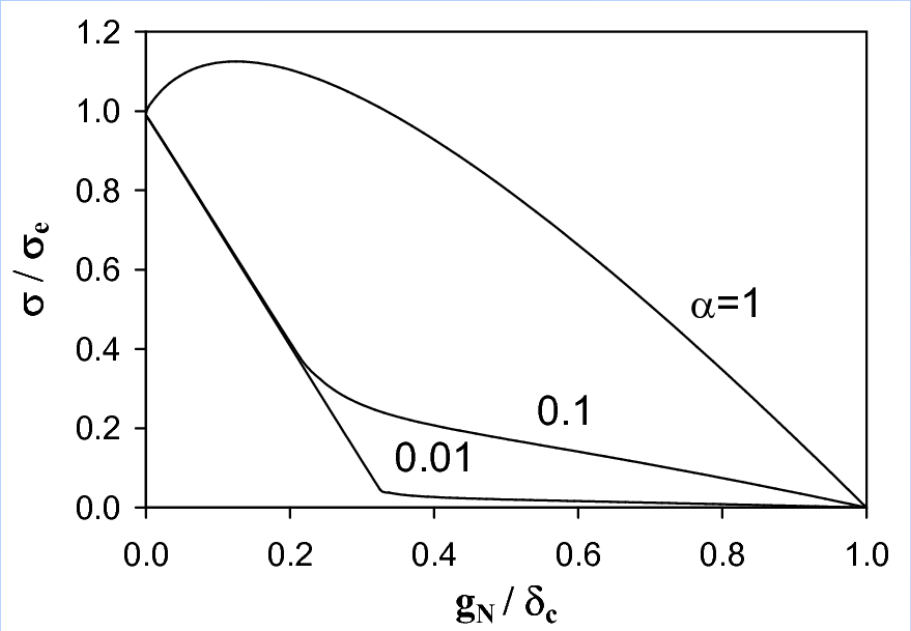
(1) How to relate the shape of the CZM to physics?

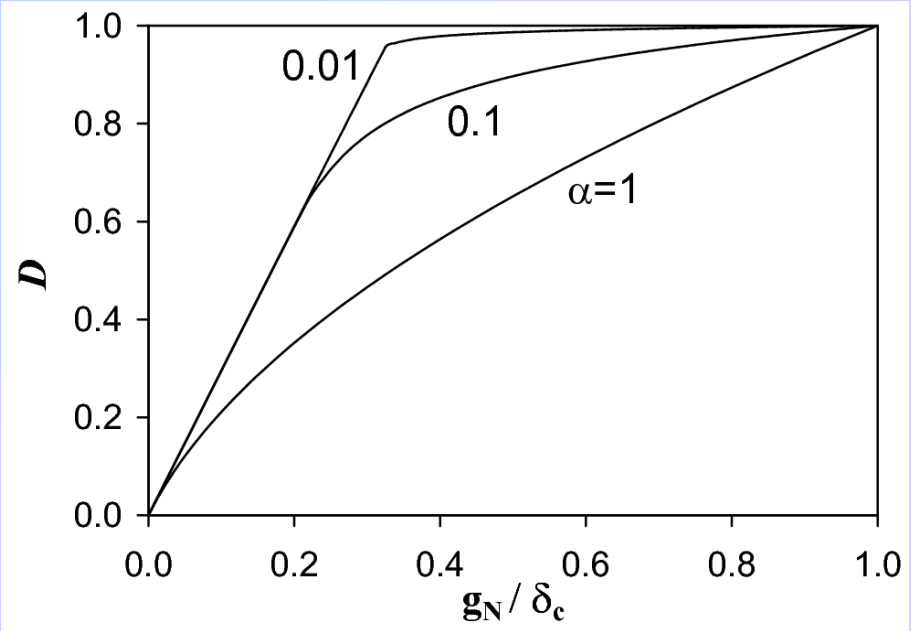
(2) How to take into account the finite thickness of real interfaces?

A nonlocal CZM for finite thickness interfaces

$$\sigma = \frac{E_2}{l_2}\frac{1-D^{\alpha}}{D^{\alpha}} g_N$$

Paggi & Wriggers (2011) **Comp. Mat. Sci.**

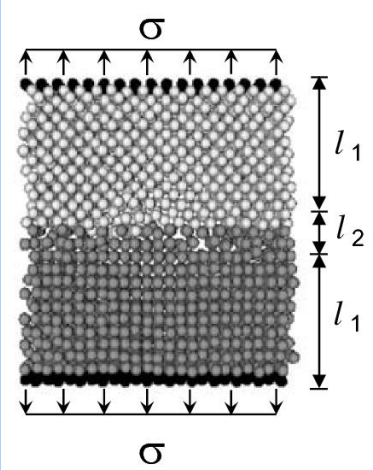




Shape of the CZM by varying α

Damage evolution

Interpretation of MD simulations

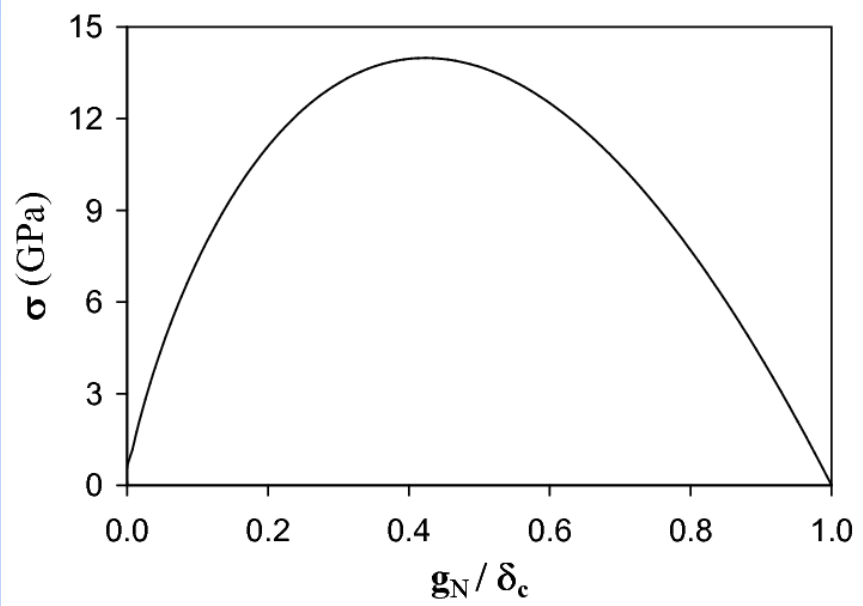


Spearot et al. (2004) **Mech. Mater.**, 36:825-847.

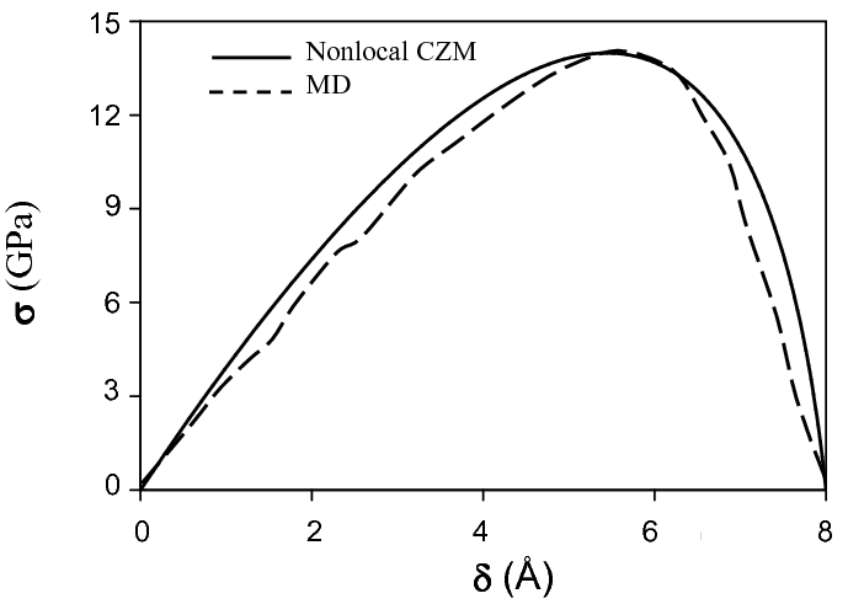
Copper (fcc crystal)

$2l_2+l_1=43.38$ Å, $E_1=E_2=110$ GPa

$\delta_e=0.2$ Å, $\delta_c=8.0$ Å, $\alpha=0.9$



Shape of the CZM



Comparison with MD

Weak form

$$\int_V (\nabla \delta \mathbf{u})^{\mathrm{T}} \boldsymbol{\sigma} \, \mathrm{d}V = \int_{\partial V} \delta \mathbf{u}^{\mathrm{T}} \mathbf{f} \, \mathrm{d}S + \int_S \delta \mathbf{g}^{\mathrm{T}} \mathbf{t} \, \mathrm{d}S$$

CZM contributions

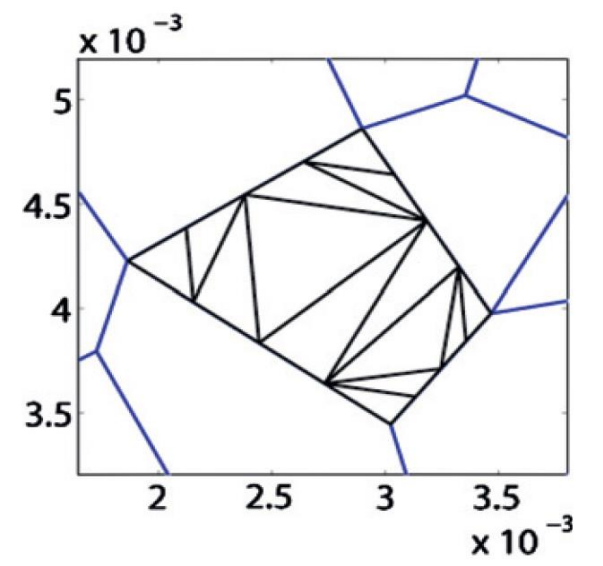
$$\int_V q \, \nabla \delta T \, \mathrm{d}V = \int_V \rho c_V \dot{T} \delta T \, \mathrm{d}V + \int_{\partial V} q_n \delta T \, \mathrm{d}S + \int_S q_s \delta T \, \mathrm{d}S$$

$$G_{\mathrm{int}} = \int_S \left(\delta g_{\mathrm{T}}, \delta g_{\mathrm{N}}, \delta \Delta T \right) \begin{pmatrix} \tau \\ \sigma \\ q_{\mathrm{S}} \end{pmatrix} \mathrm{d}S$$

$$\Delta G_{\mathrm{int}} = \int_S \left(\delta g_{\mathrm{T}}, \delta g_{\mathrm{N}}, \delta \Delta T \right) \mathbf{C} \begin{pmatrix} g_{\mathrm{T}} \\ g_{\mathrm{N}} \\ \Delta T \end{pmatrix} \mathrm{d}S$$

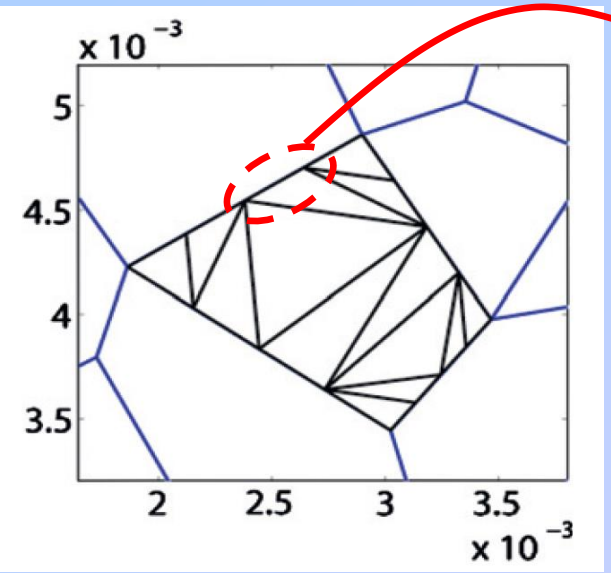
$$\mathbf{C} = \begin{bmatrix} \dfrac{\partial \tau}{\partial g_{\mathrm{T}}} & \dfrac{\partial \tau}{\partial g_{\mathrm{N}}} & 0 \\ \dfrac{\partial \sigma}{\partial g_{\mathrm{T}}} & \dfrac{\partial \sigma}{\partial g_{\mathrm{N}}} & 0 \\ 0 & \dfrac{\partial q_{\mathrm{S}}}{\partial g_{\mathrm{N}}} & \dfrac{\partial q_{\mathrm{S}}}{\partial \Delta T} \end{bmatrix}$$

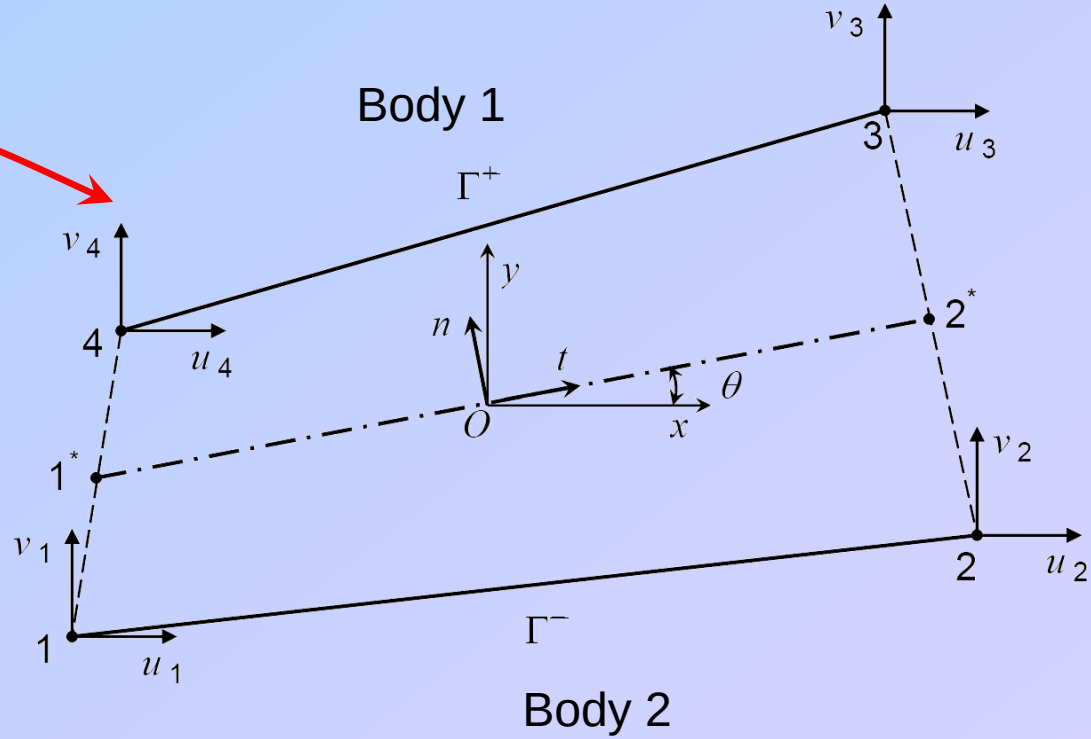
Finite element implementation in FEAP



M. Paggi, P. Wriggers: "A nonlocal cohesive zone model for finite thickness interfaces – Part II: FE implementation and application to polycrystalline materials", **Comp. Mat. Sci.**, Vol. 50 (5), 1634-1643, 2011.

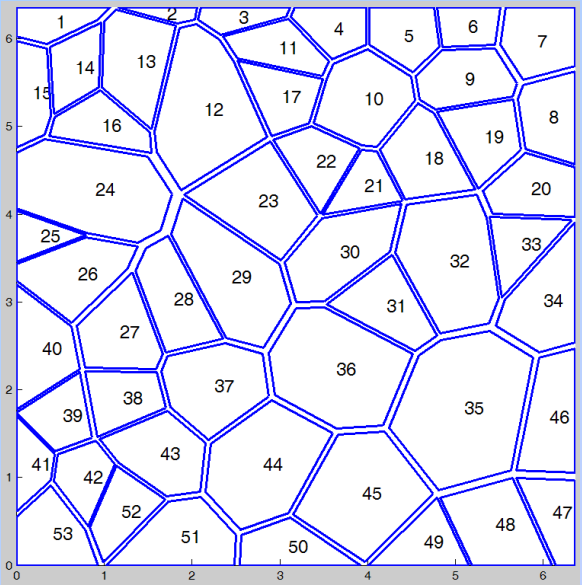
Finite element implementation in FEAP

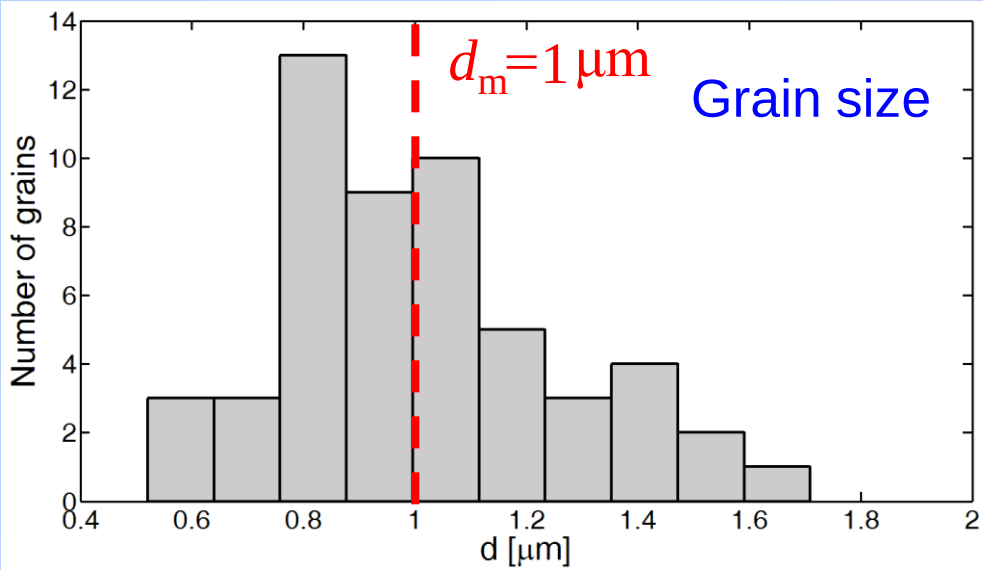


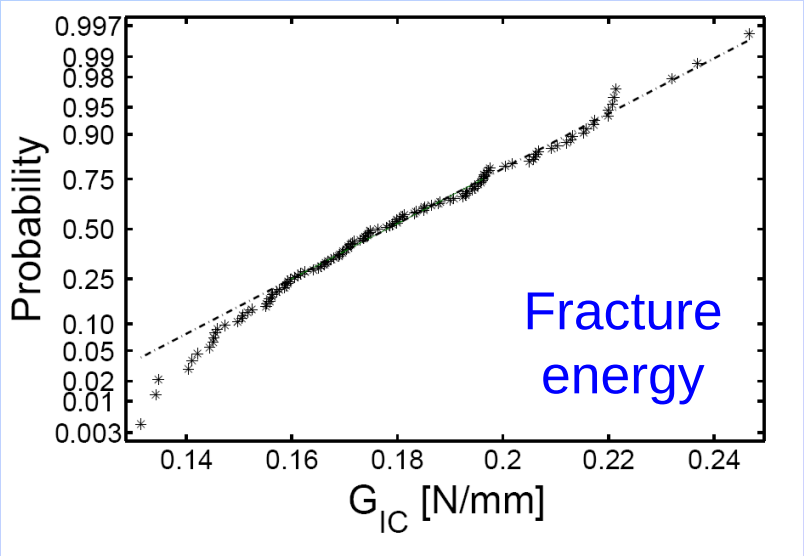


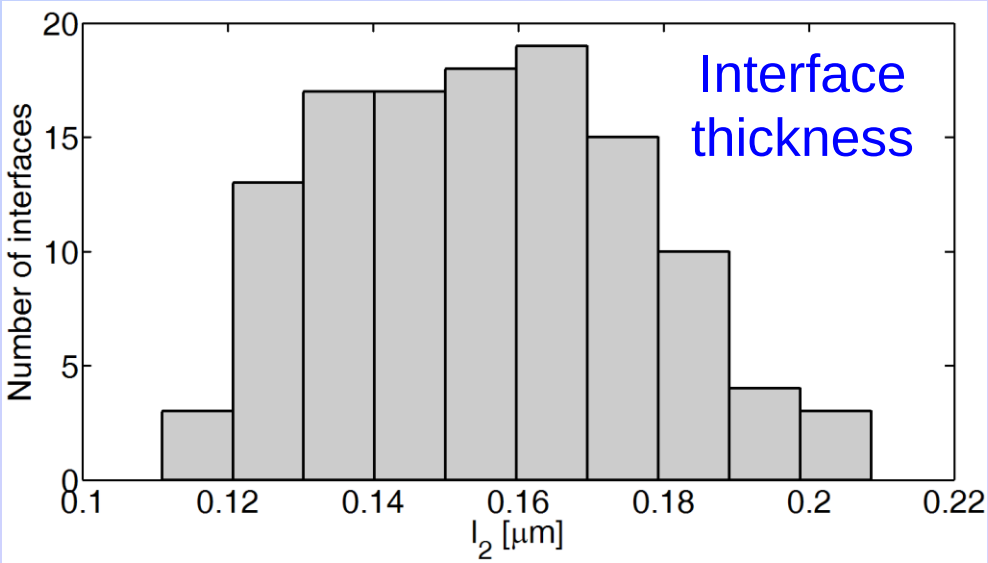
M. Paggi, P. Wriggers: "A nonlocal cohesive zone model for finite thickness interfaces – Part II: FE implementation and application to polycrystalline materials", **Comp. Mat. Sci.**, Vol. 50 (5), 1634-1643, 2011.

Application to polycrystalline materials

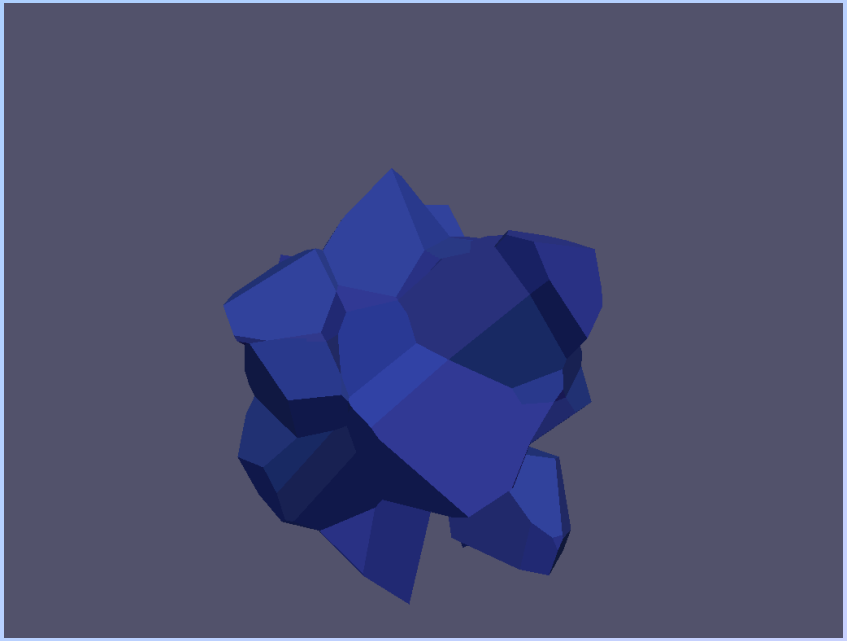




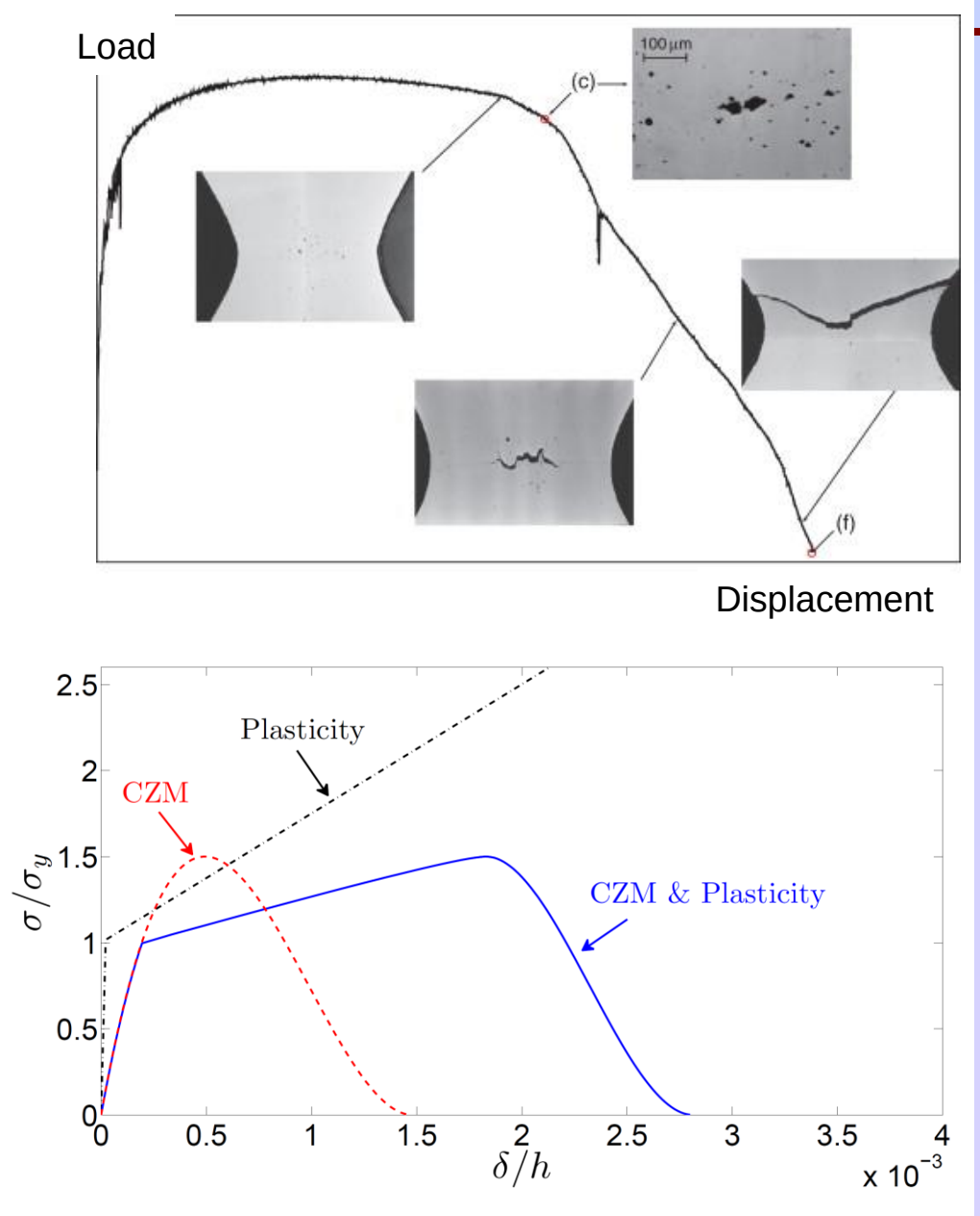




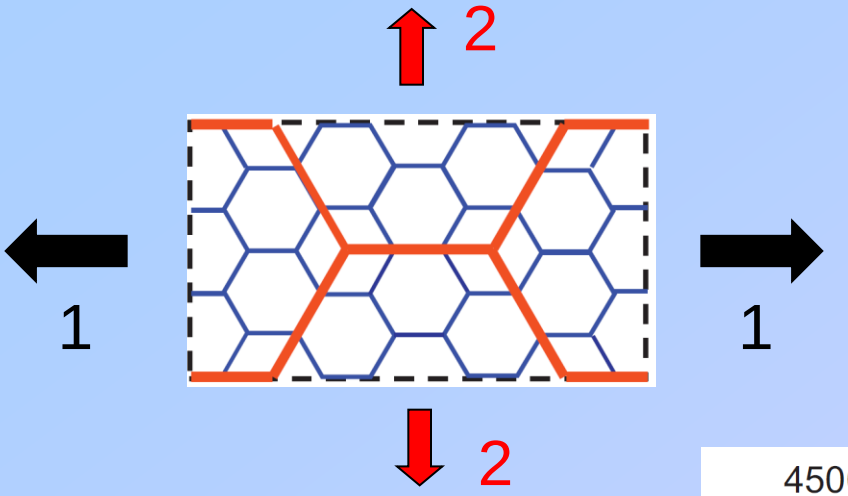
3D Virtual tensile test

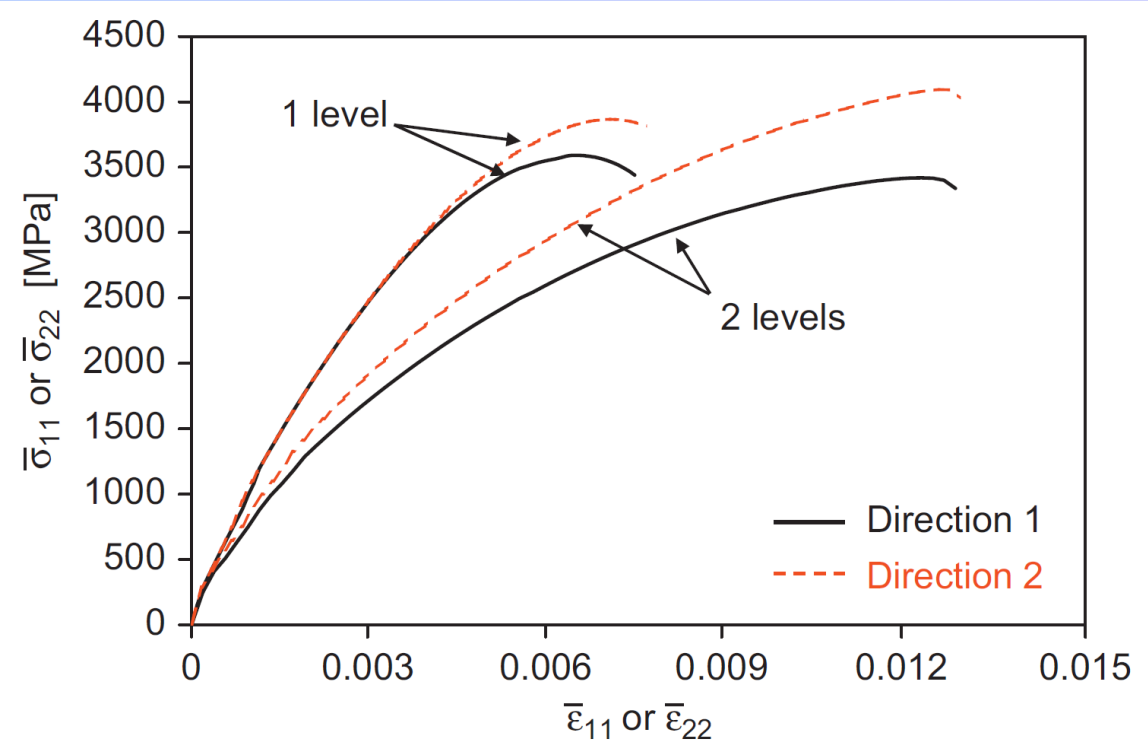


Paggi, Lehmann, Weber, Carpinteri, Wriggers (2012)

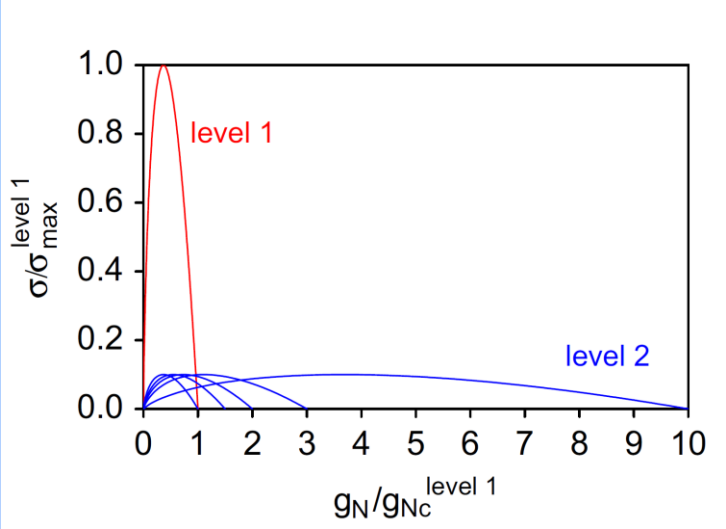


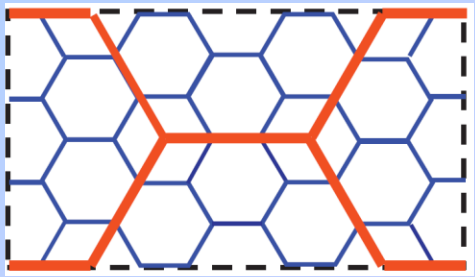
Effect of hierarchy on anisotropy

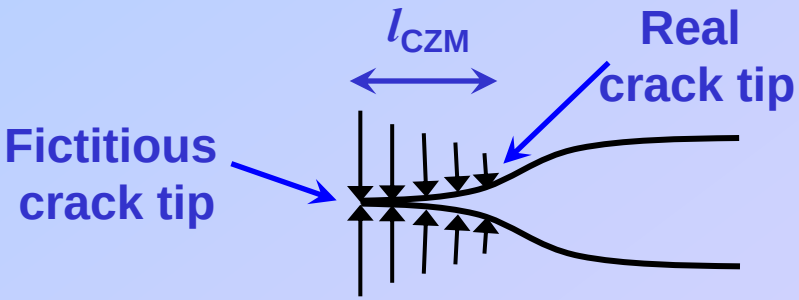




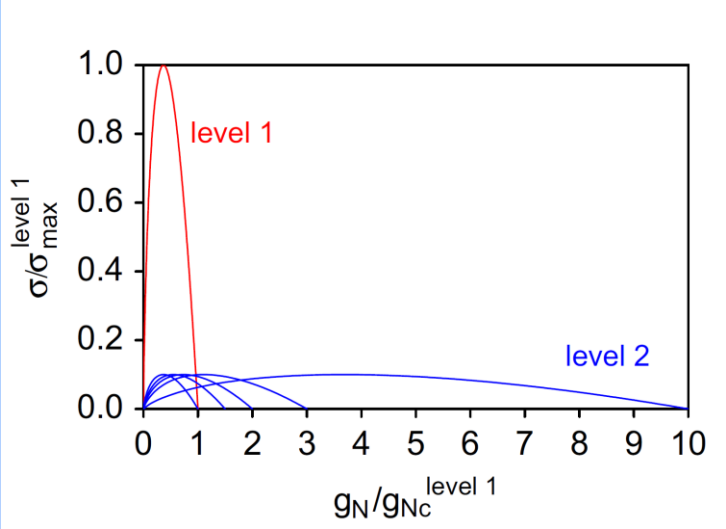
Effect of hierarchy on strength

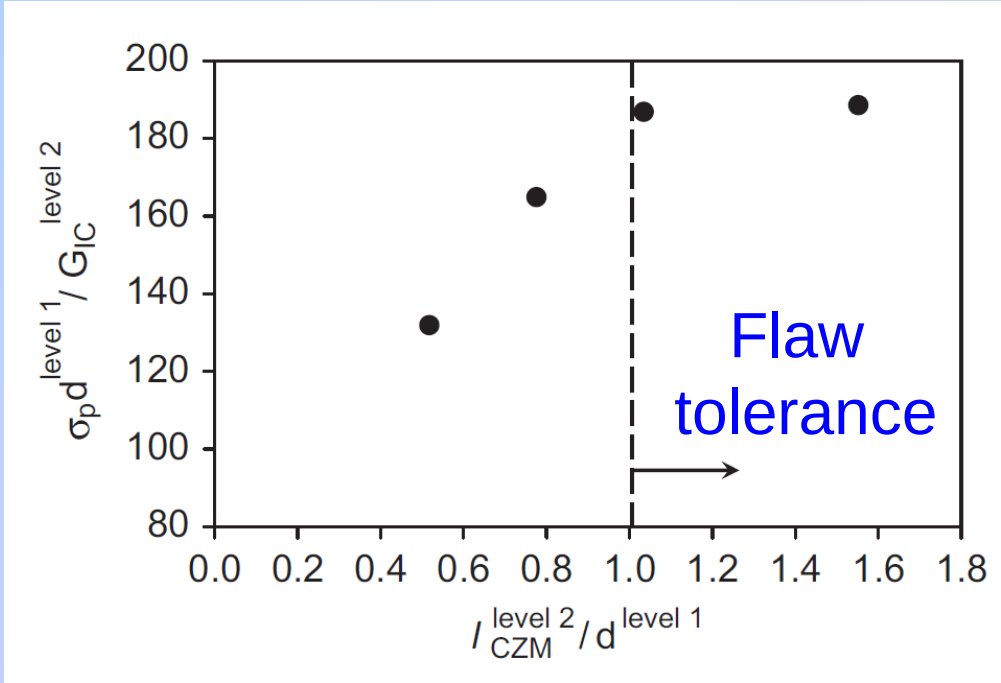


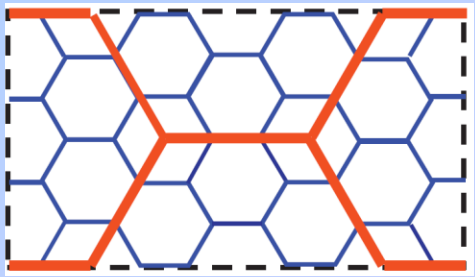


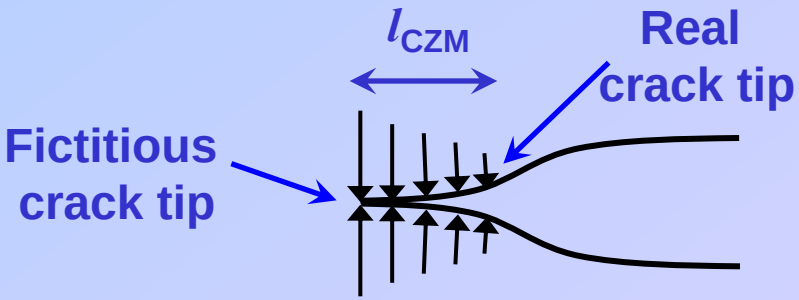


Effect of hierarchy on strength





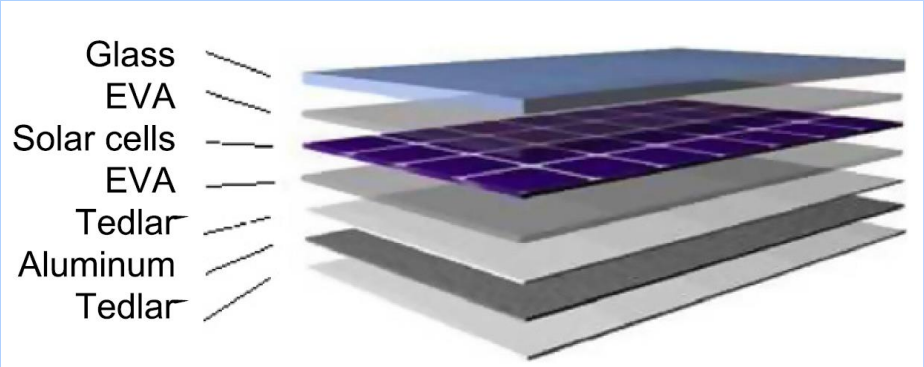


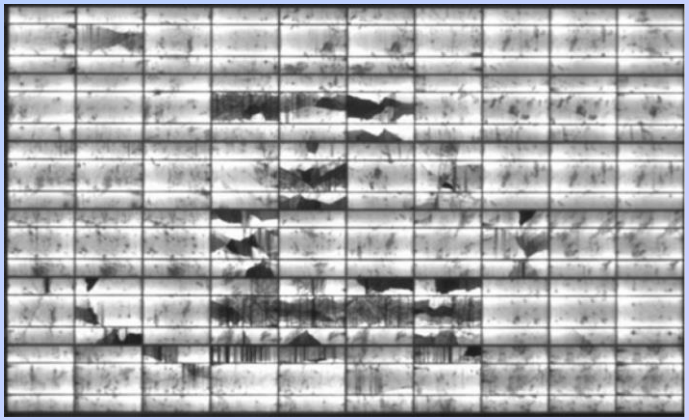


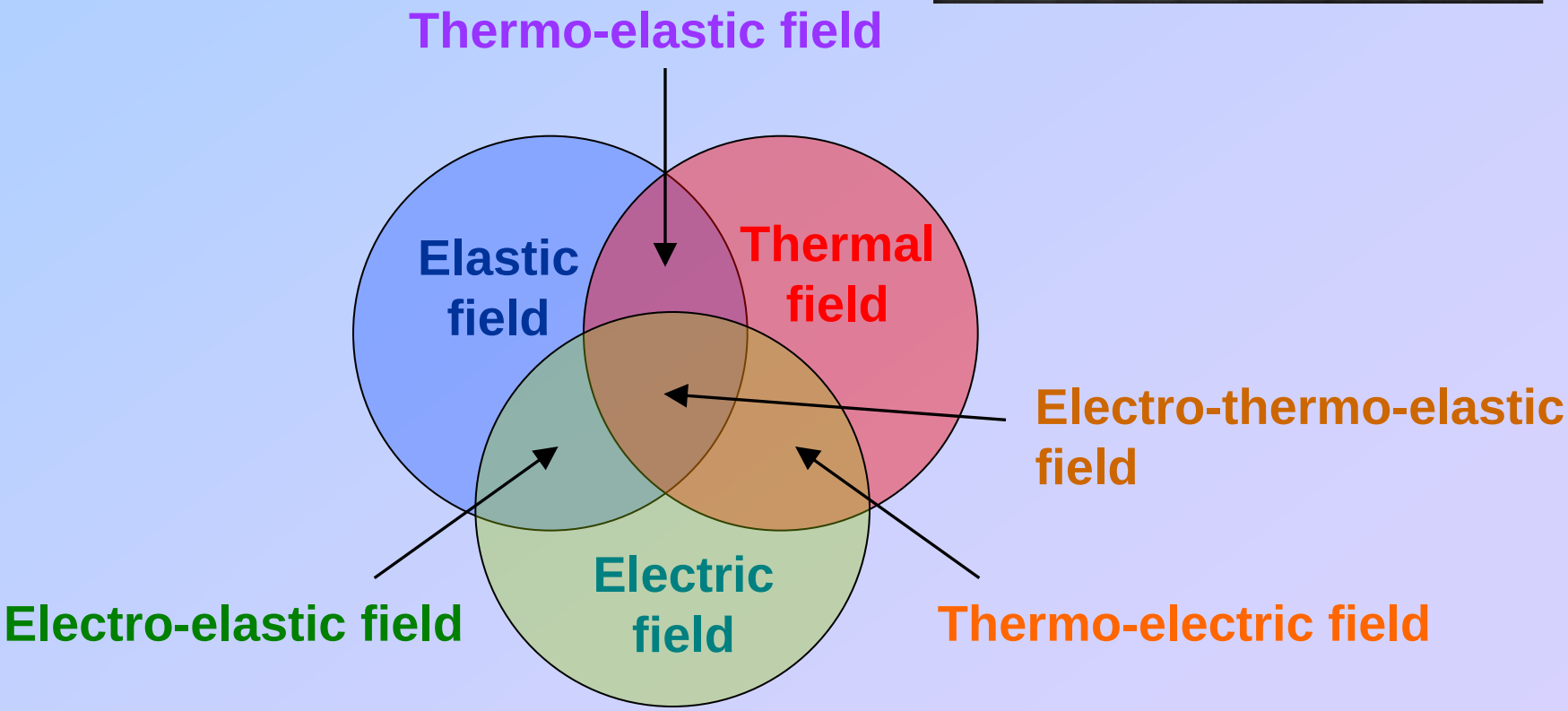
l_{CZM} = process zone size for the grain boundaries of the level 2

$d^{level\ 1}$ = diameter of the rods (level 1)

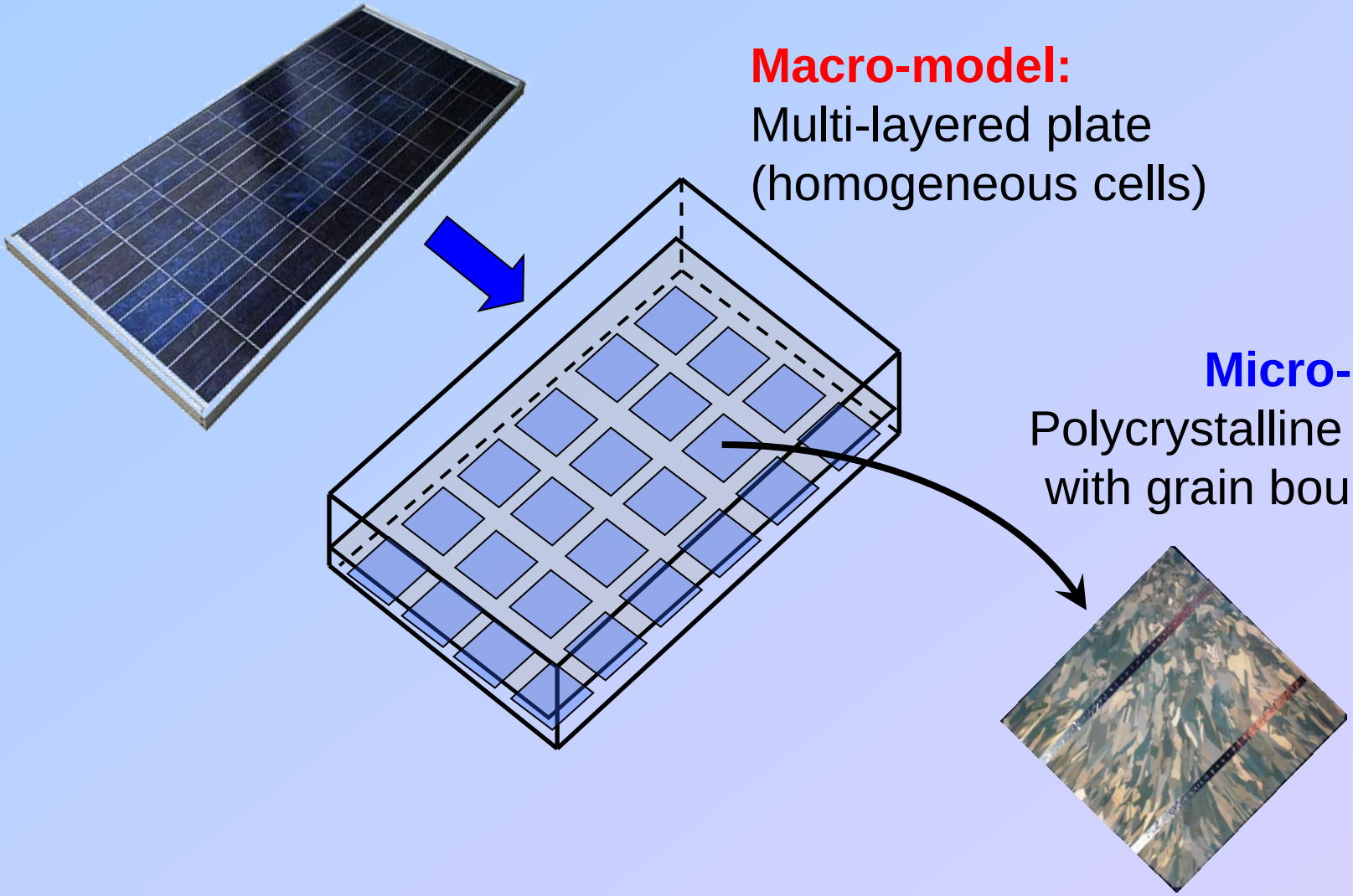
Interfaces in multiphysics





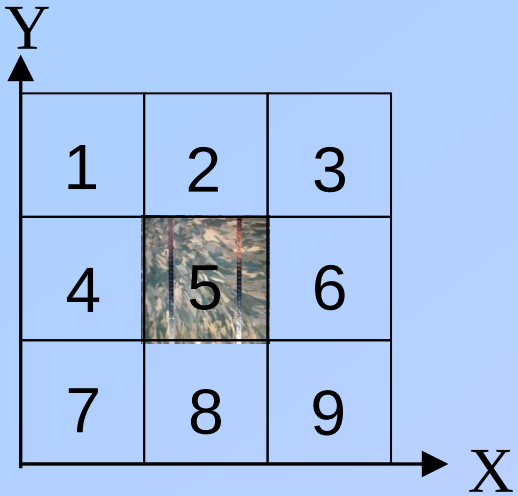


A multiscale solution strategy

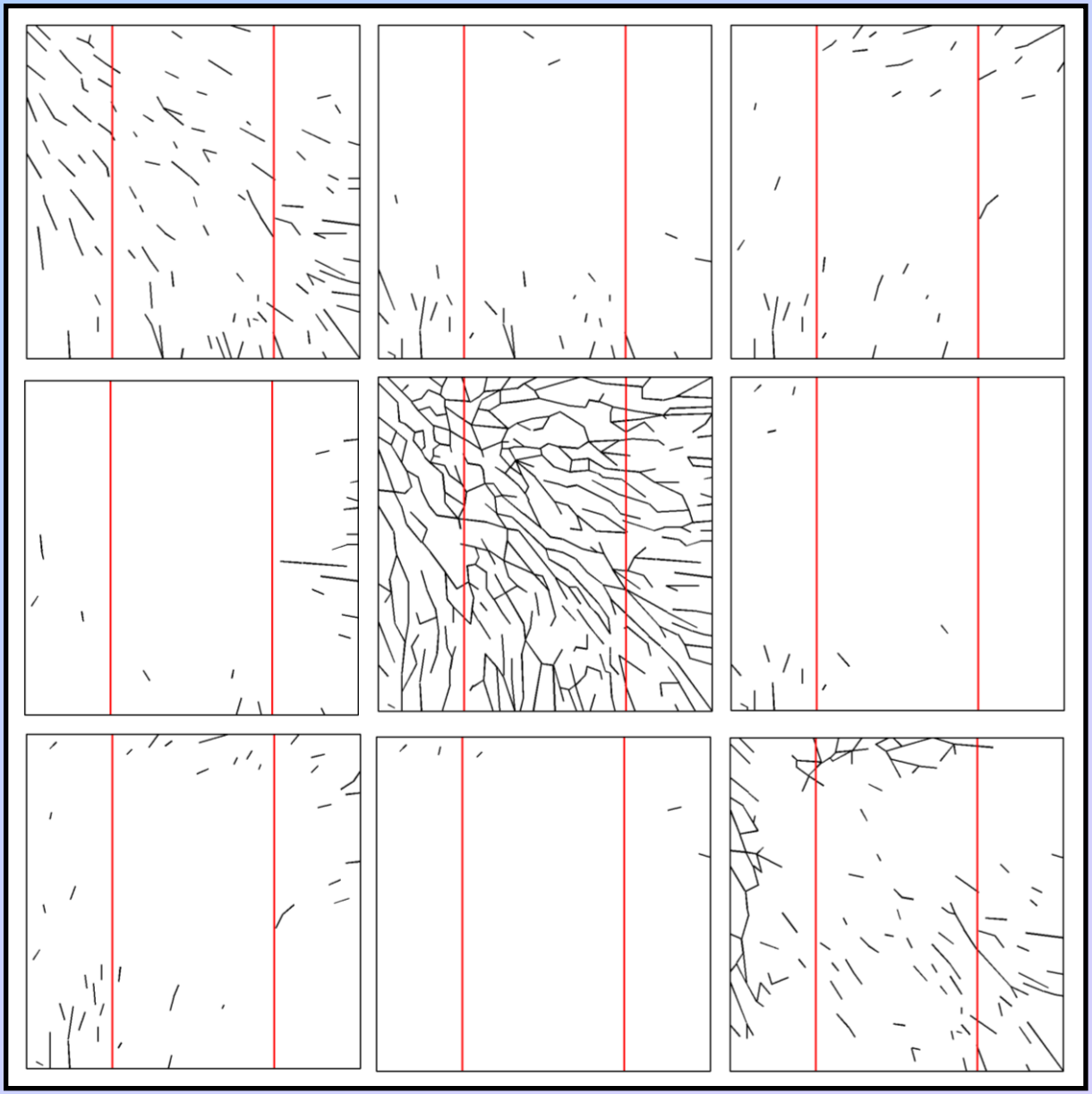


M. Paggi, M. Corrado, M.A. Rodriguez (2013)
Composite Structures, 95:630-638.

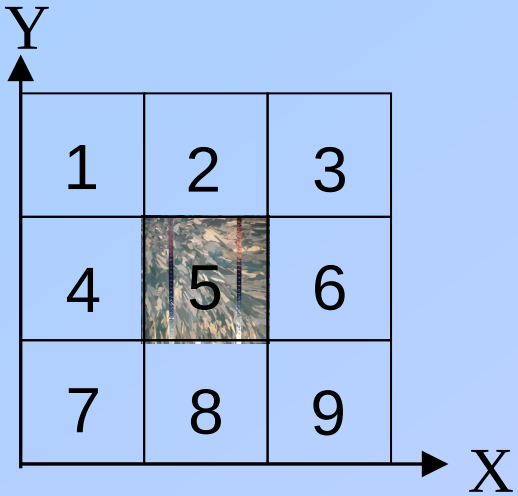
Micro-crack pattern in Silicon cells



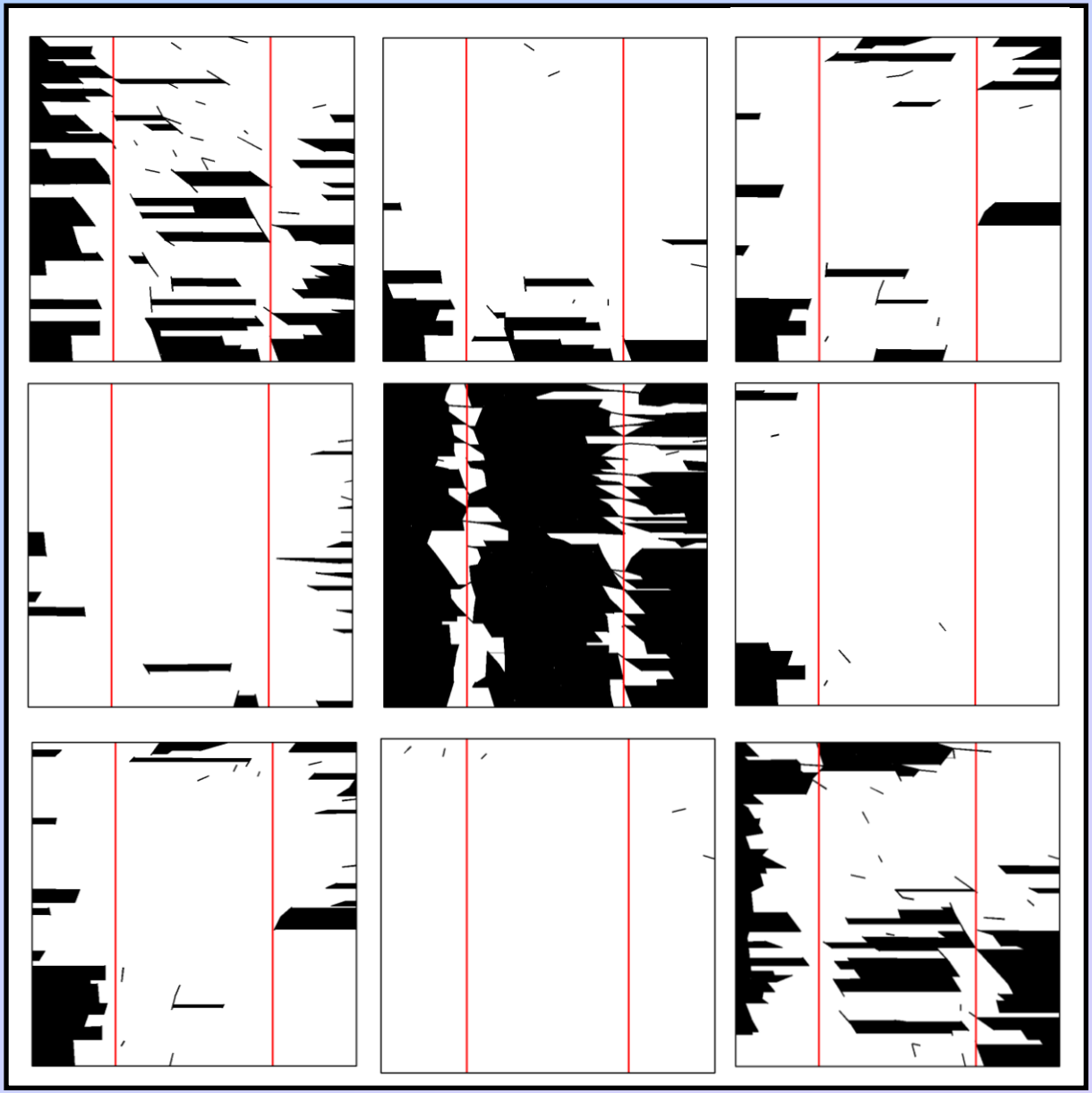
Simply supported plate subjected to a pressure of 5400 Pa



Electrically inactive areas



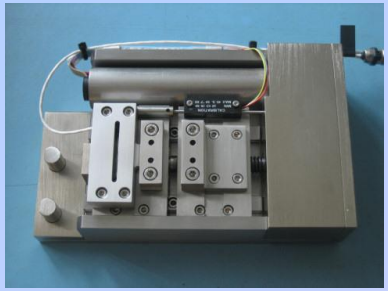
Simply supported plate subjected to a pressure of 5400 Pa



Centre for Risk Analysis and Durability of Structures

3D confocal-interferometric profilometer (LEICA, DCM 3D)

SEM (ZEISS, EVO MA15)



Testing stage (DEBEN, 5000S)

erc
European Research Council
Established by the European Commission

Thermocamera (FLIR, T640bx)

Photocamera for EL tests (PCO, 1300 Solar)

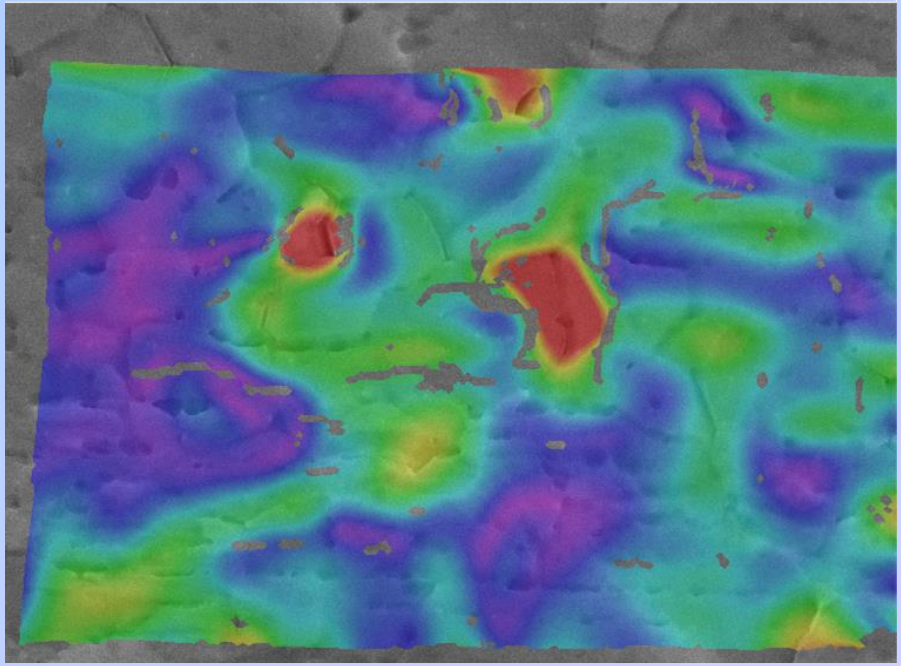
Testing machine & thermostatic chamber (Zwick/Roell, Z010TH)

Server HP Proliant DL585R07

Ongoing research topics

Determination of interface properties via inverse analysis of microstructure evolution of polycrystals during a tensile tests

(with Dr. M. Schaper, Lebniz University Hannover)

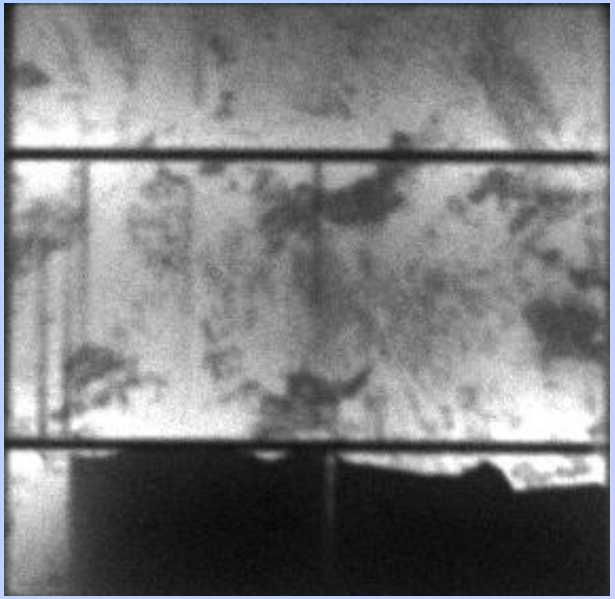


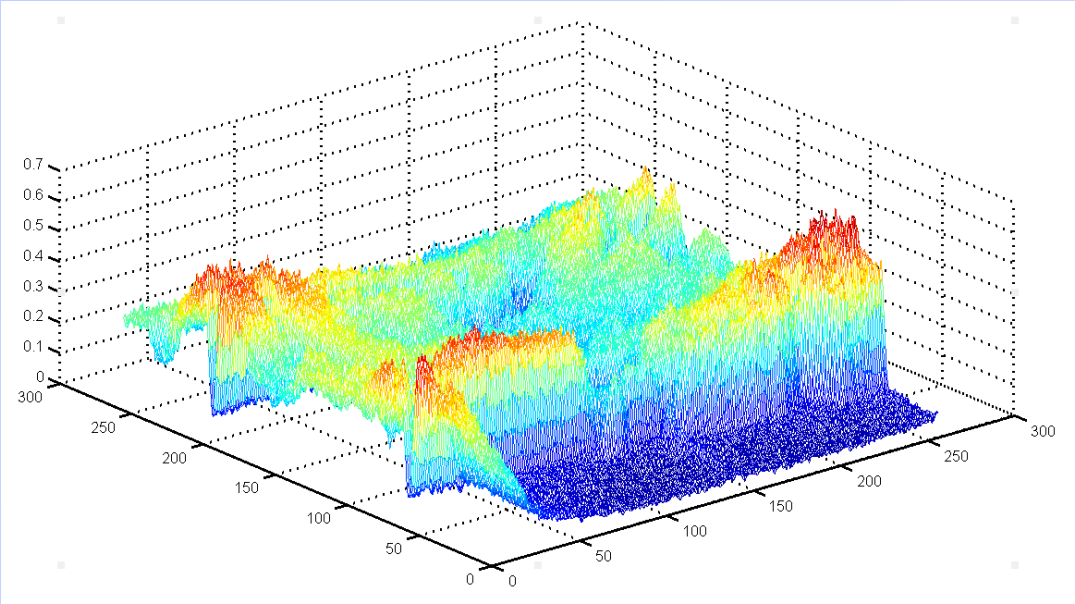
SEM image with superimposed digital image correlation of the strain field

Ongoing research topics

Quantitative analysis of EL images via fractal concepts and spectral methods

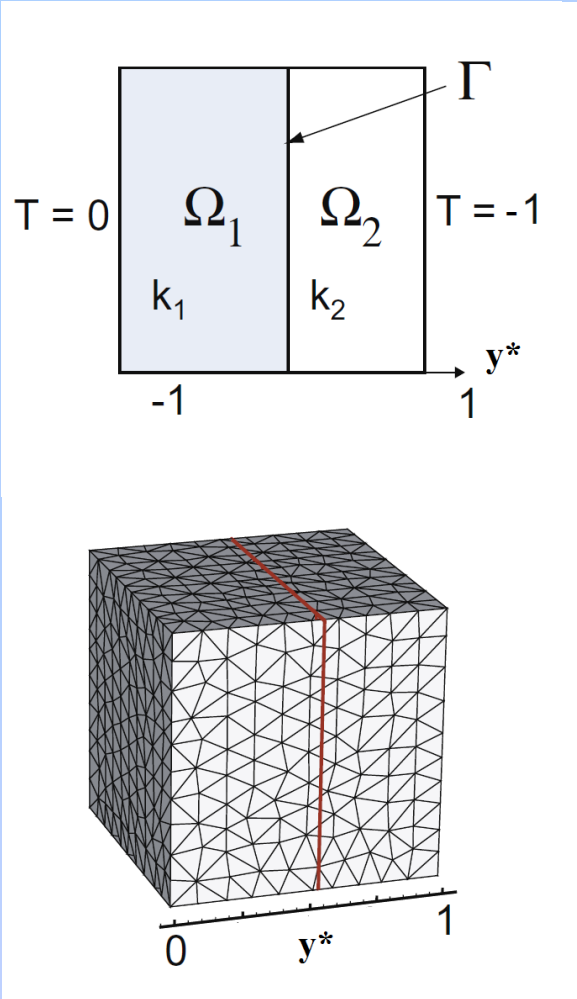
(with Ing. I. Berardone & ISFH)

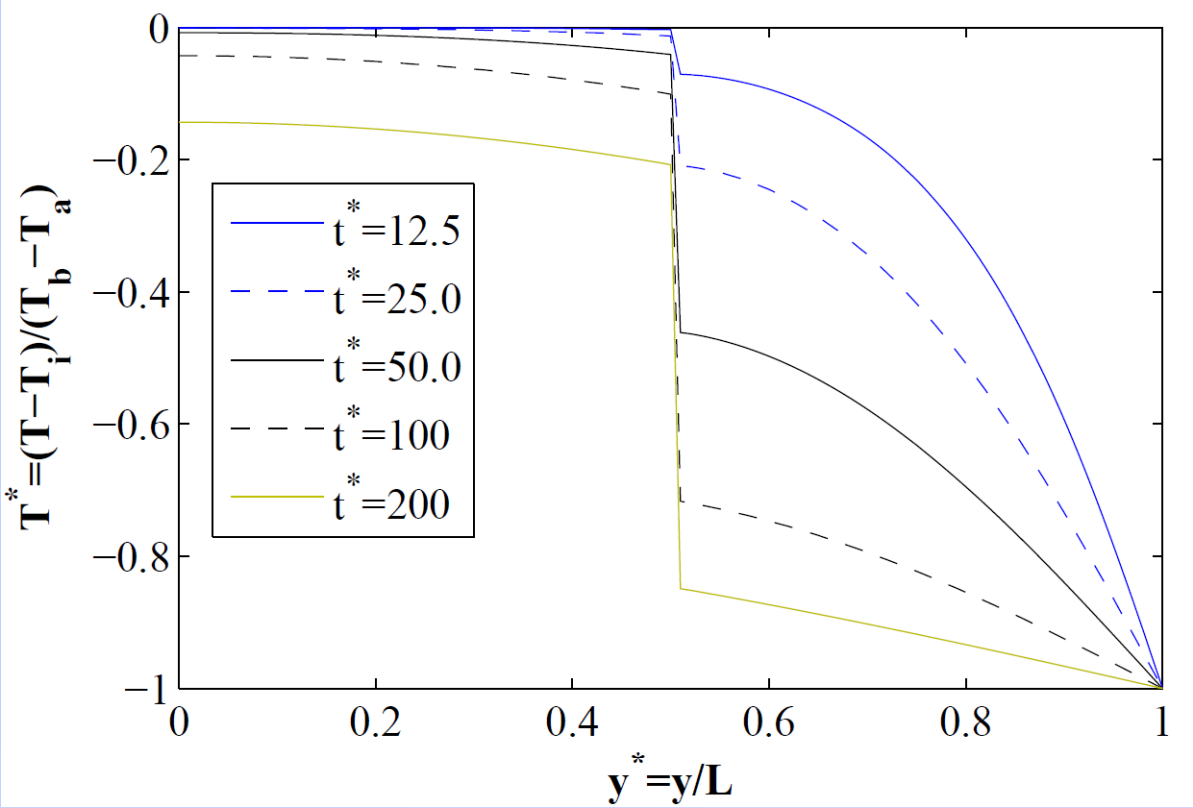




EL image of a microcracked Silicon cell

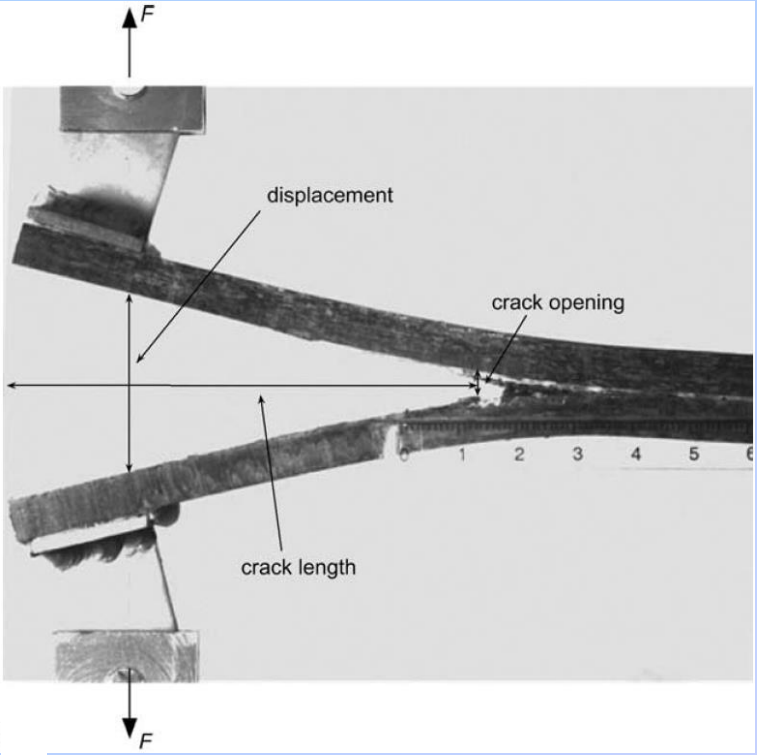
Ongoing research topics

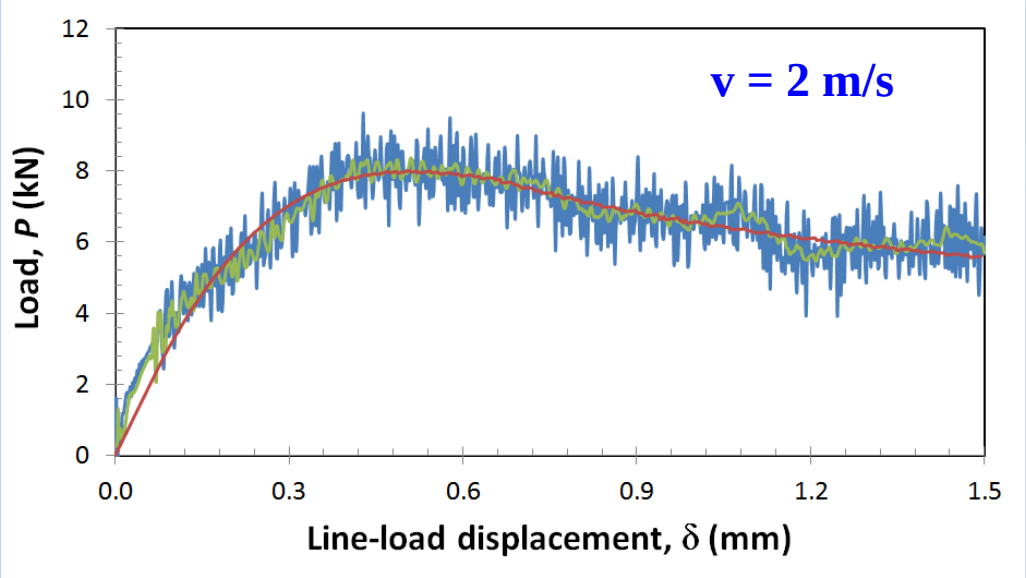




Thermoelastic cohesive zone models (with Dr. A. Sapora)

Ongoing research topics





Nonlinear crack propagation in dynamics
(with Dr. M. Corrado)