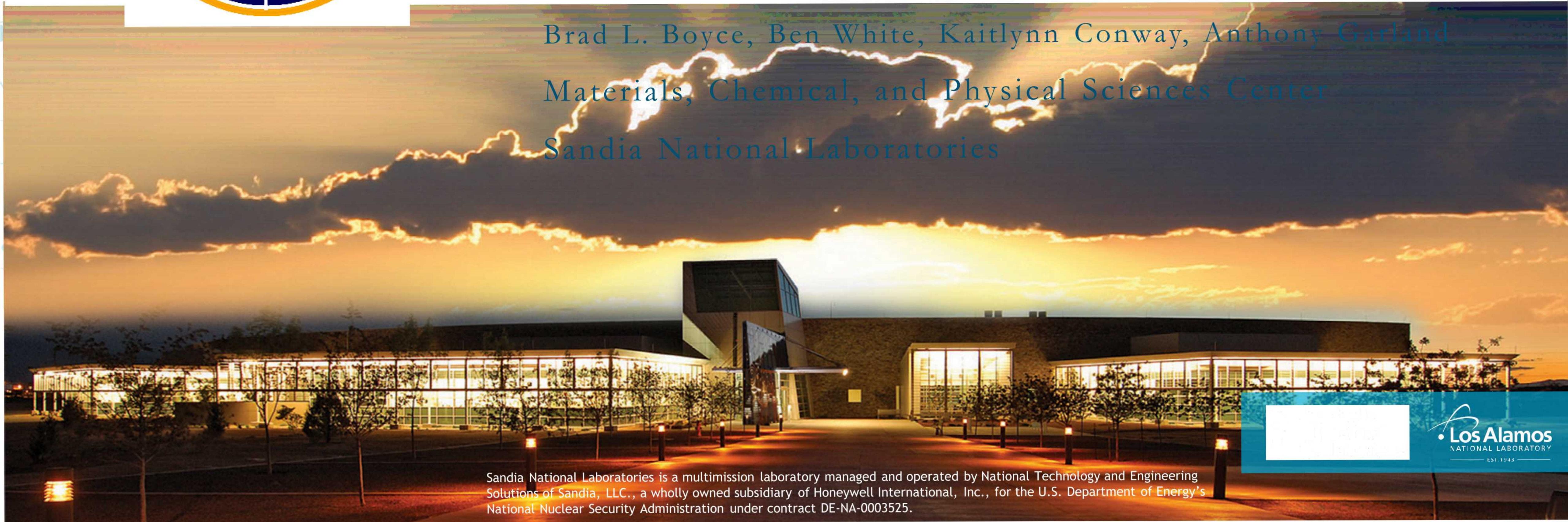
SAND2020-9684C

Toughening materials with air?



Brad L. Boyce, Ben White, Kaitlynn Conway, Anthony Garland

Materials, Chemical, and Physical Sciences Center

Sandia National Laboratories

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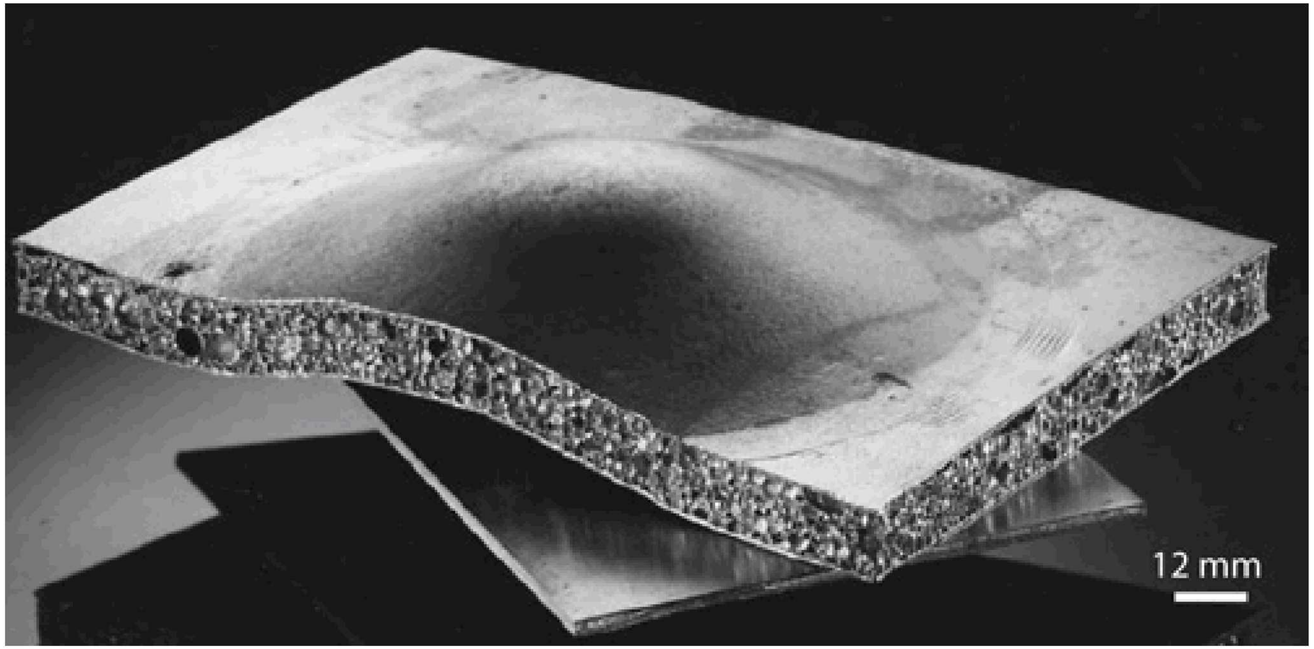
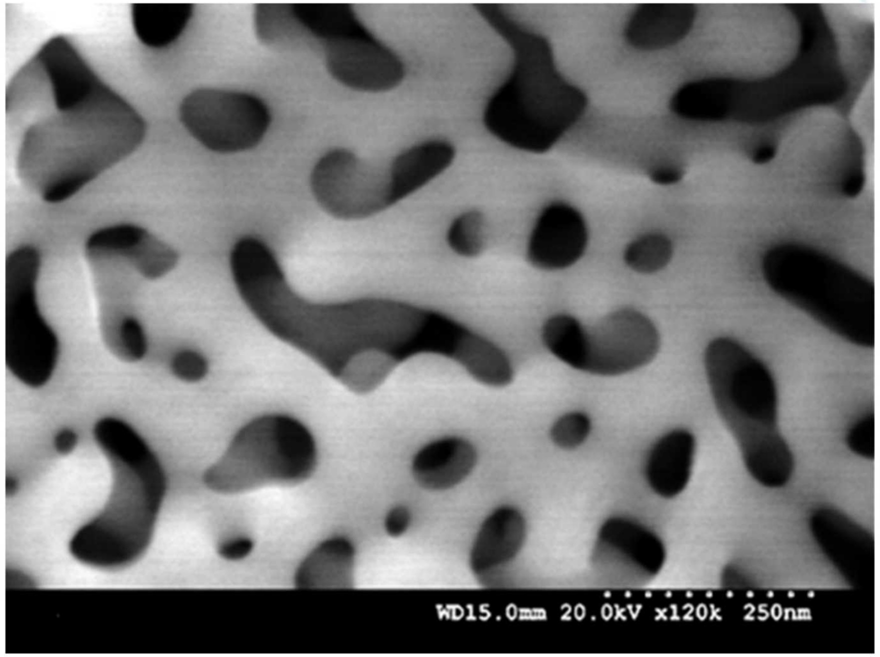
Structural metal foams… aka cellular solids



Aluminum Foam Sandwich (AFS) Panel

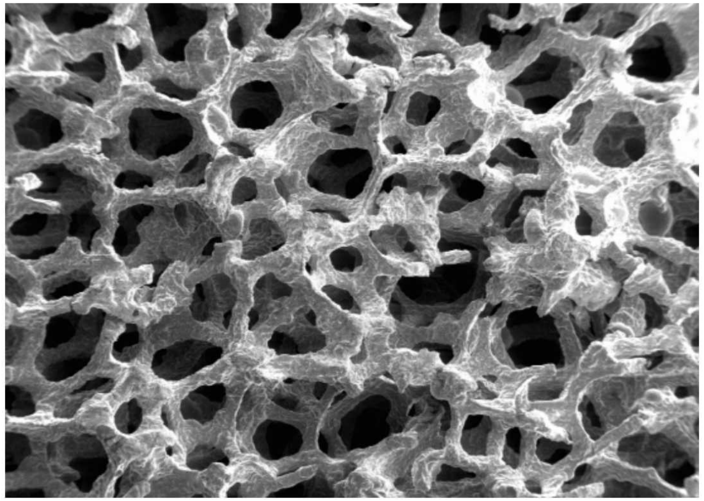


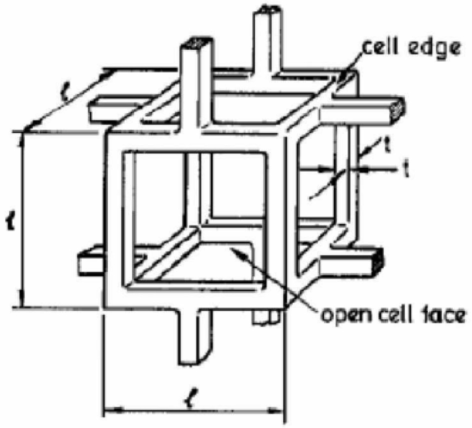
Nanoporous Au

Gold with only **one fourth the fracture toughness of glass!**

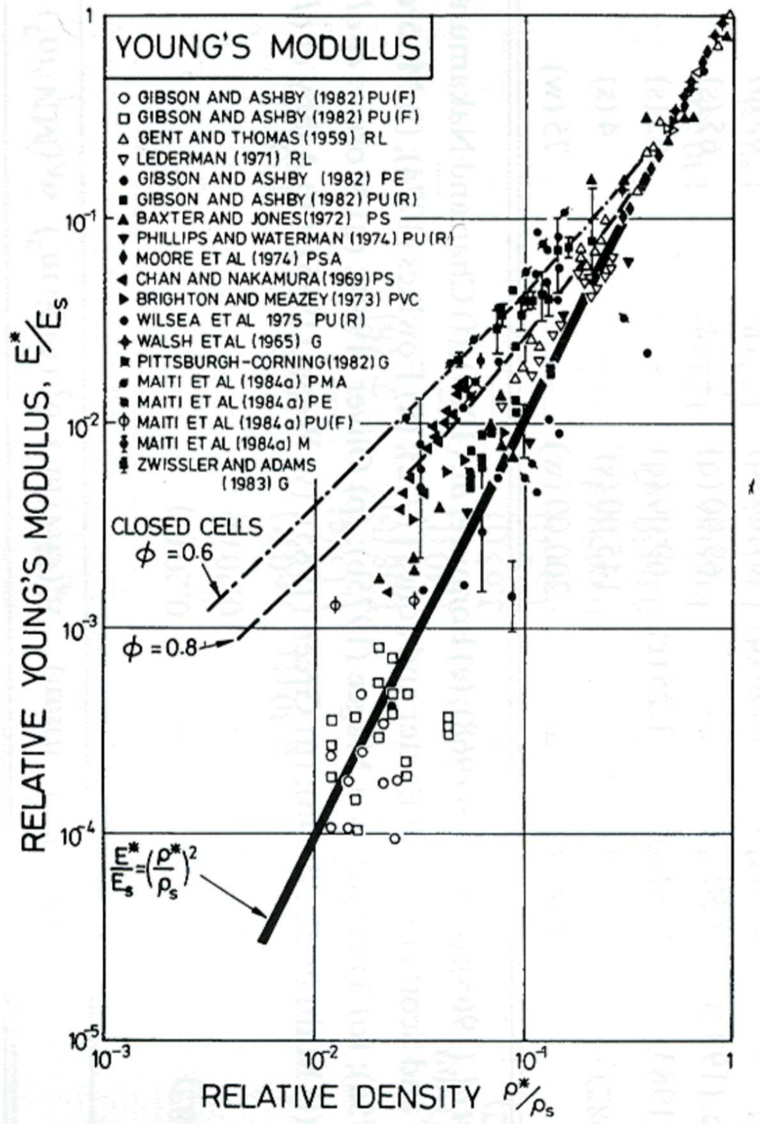
Briot, Kennerknecht, Eberl, Balk, *Phil. Mag.*, 2014

Modulus



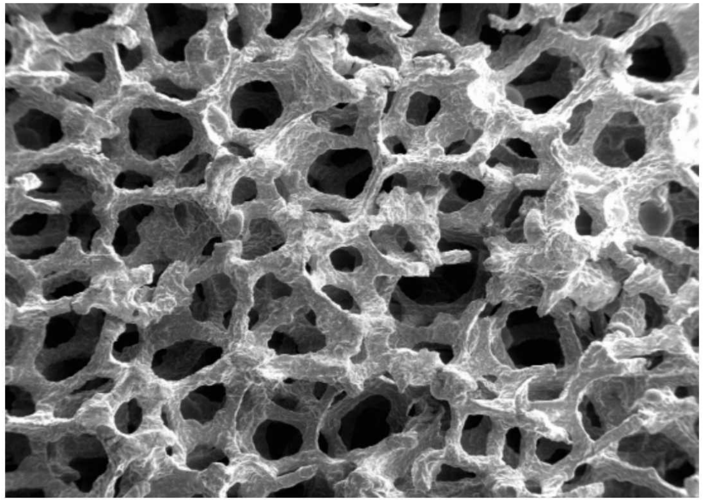


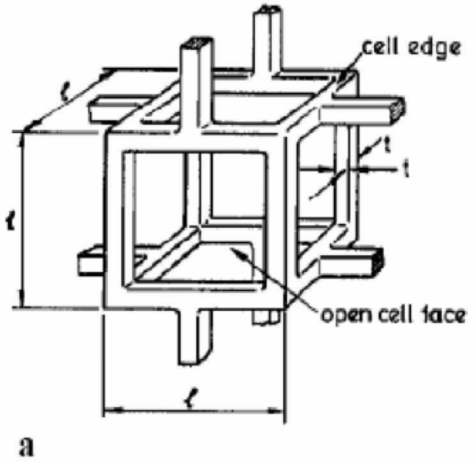
a

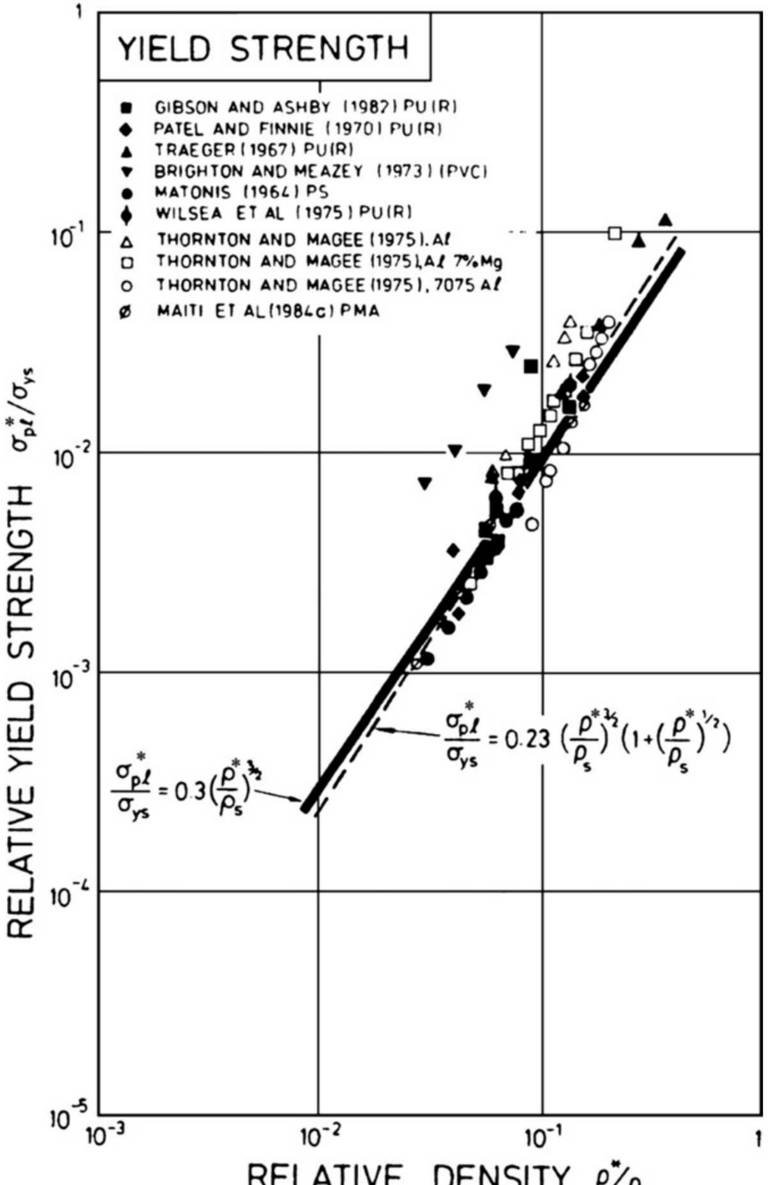


Gibson and Ashby, Cellular Solids, 1997

Strength

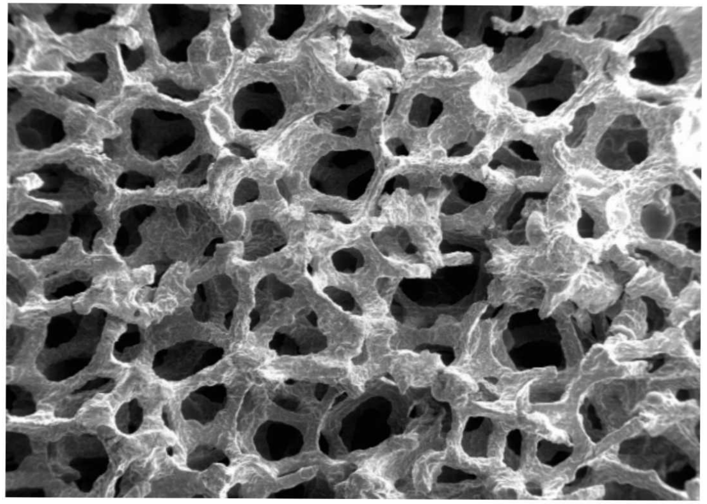


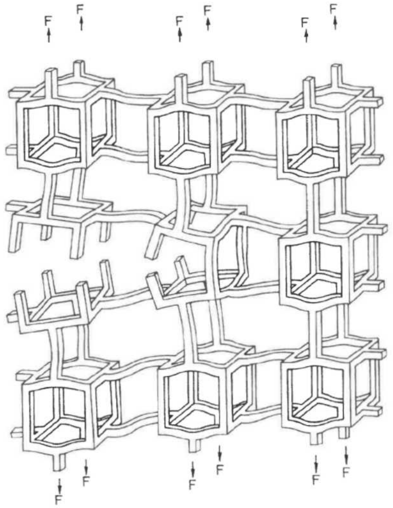


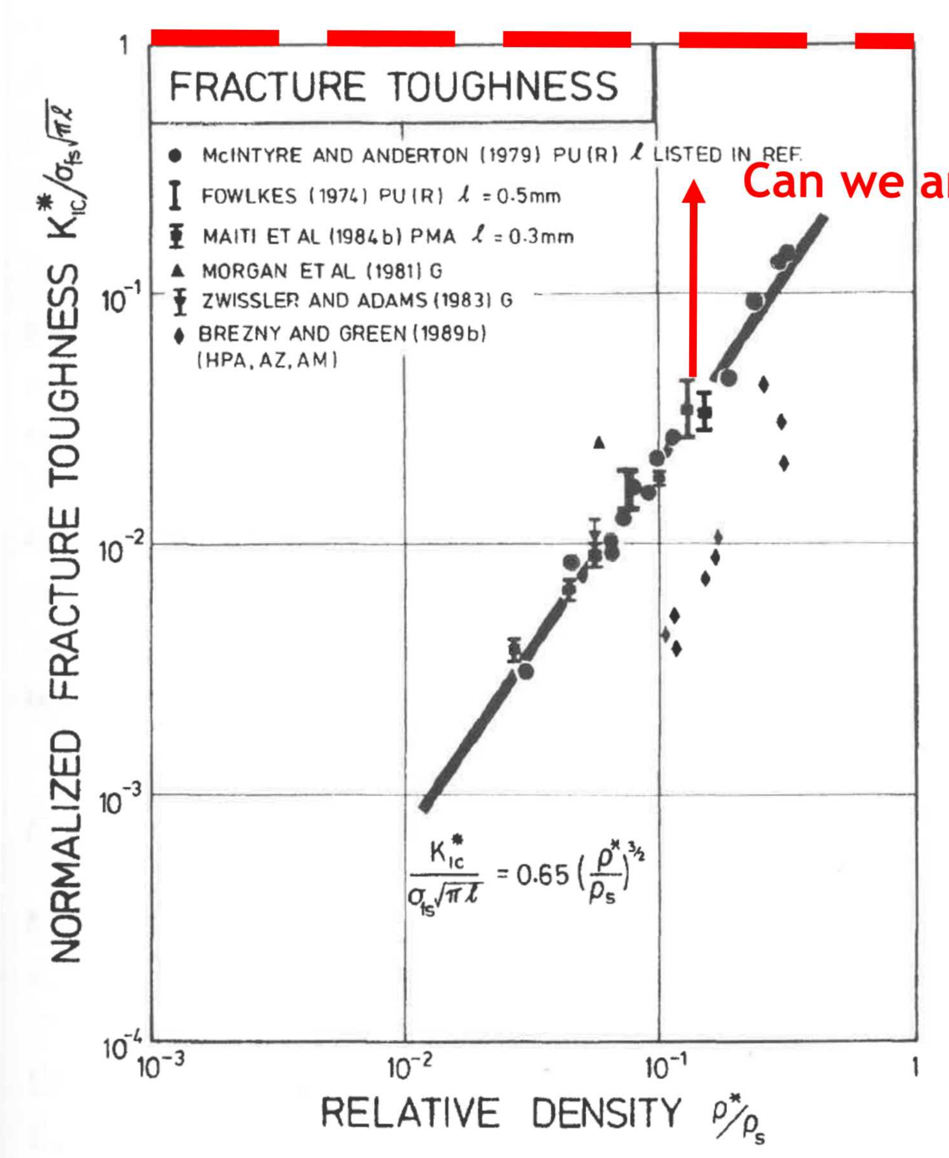


Gibson and Ashby, Cellular Solids, 1997

Foams are expected to lose toughness as density decreases







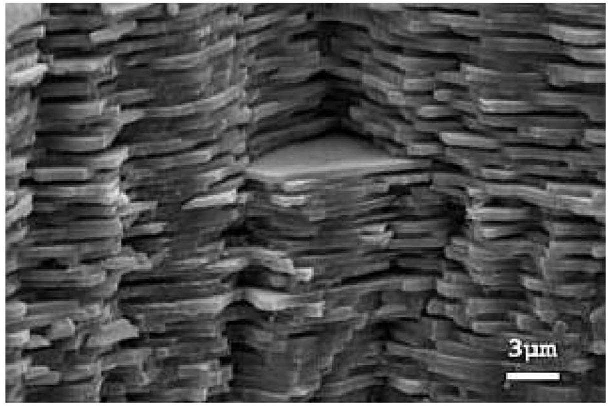
Is 1 an upper limit???

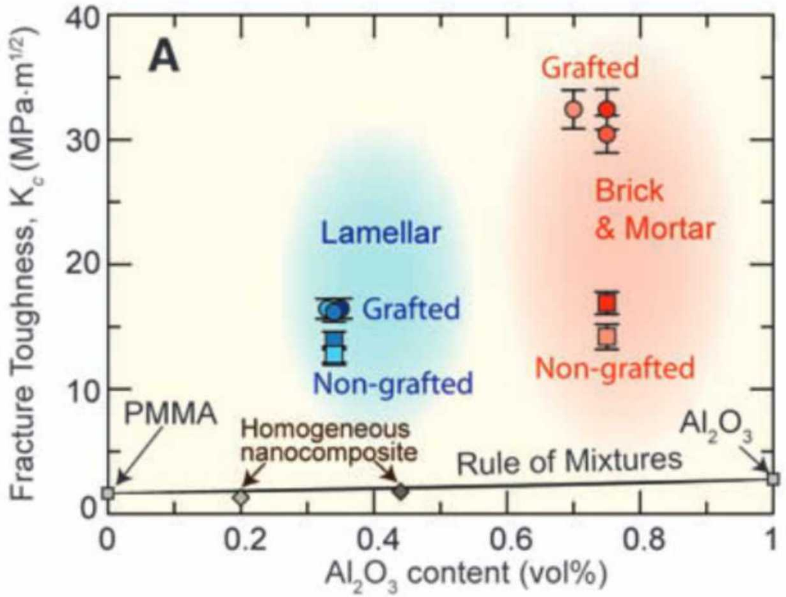
Can we architect?

Gibson and Ashby, Cellular Solids, 1997

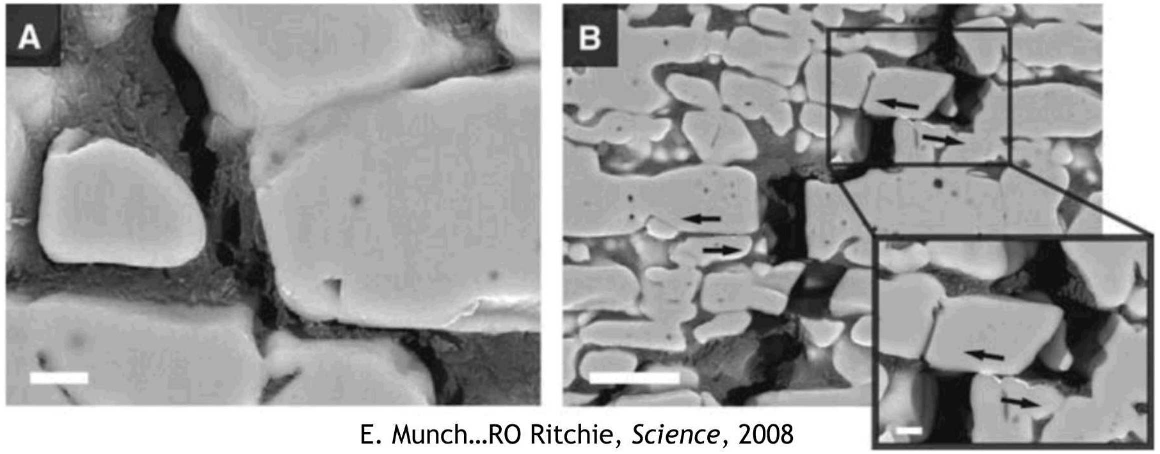
An inspiring example: synthetic nacre

Mother of pearl is mostly brittle calcium carbonate. How is it so tough???



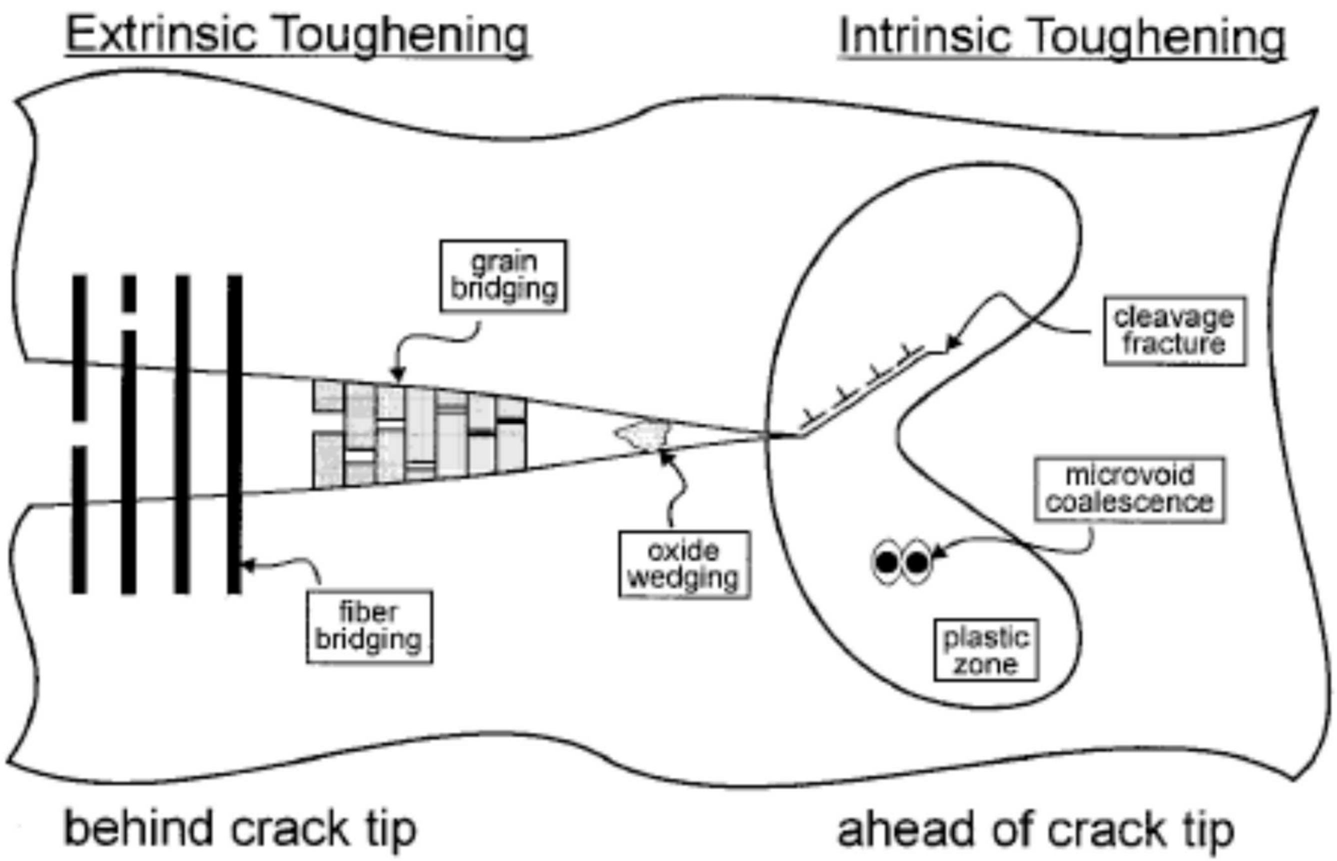


"Brick and Mortar" toughening in Synthetic Nacre



E. Munch…RO Ritchie, *Science*, 2008

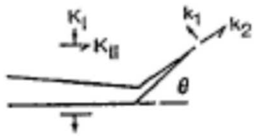
How do we improve a materials resistance to crack propagation?



RO Ritchie, *Int. J. Fracture*, 1999

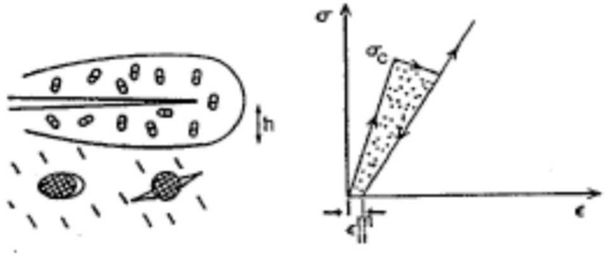
Extrinsic toughening mechanisms for brittle materials

- CRACK DEFLECTION



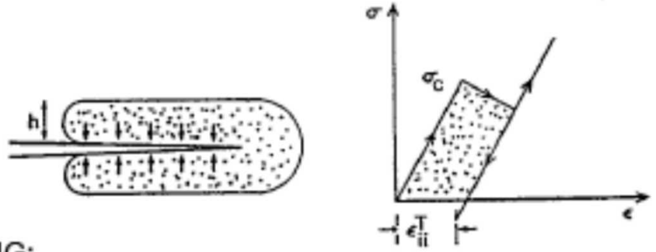
- MICROCRACK TOUGHENING:

$$\Delta(K) \sim E' f_v \, \varepsilon_{ii}^{m} \sqrt{h}$$



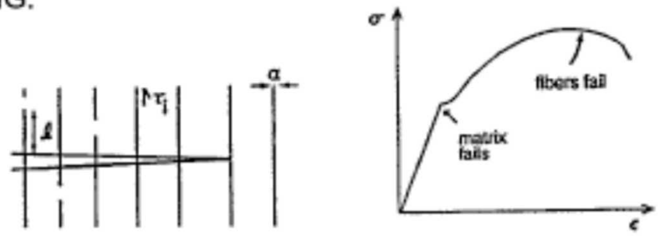
- TRANSFORMATION TOUGHENING:

$$\Delta(K) \sim E' f_v \, \varepsilon_{ii}^{T} \sqrt{h}$$



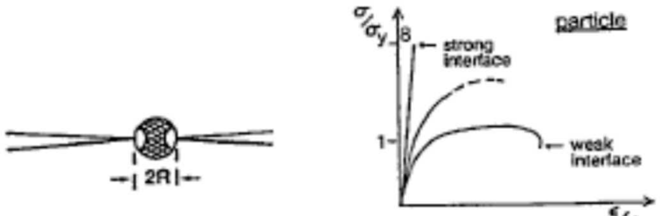
- BRITTLE FIBER/WHISKER TOUGHENING:
(crack bridging)

$$\Delta(K) \sim \left(2 f_v E' \tau_i \ell^2 / \alpha\right)^{1/2}$$



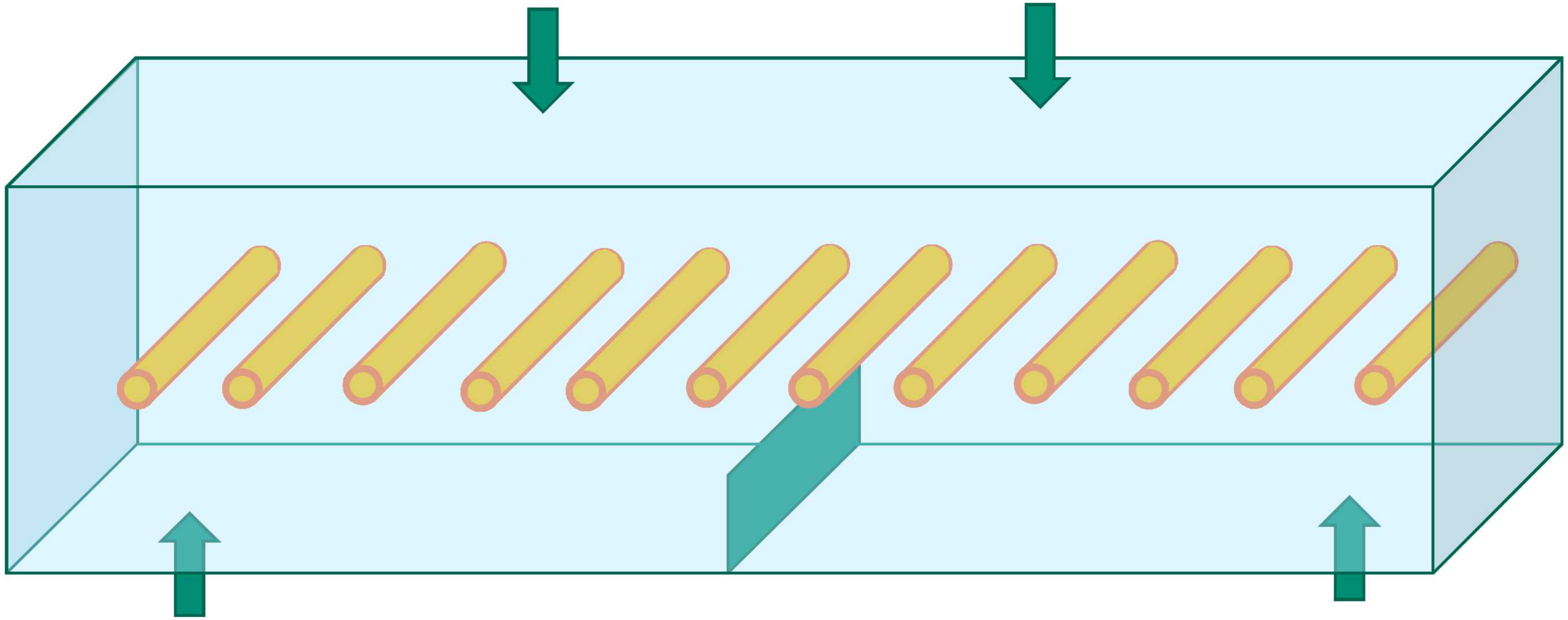
- DUCTILE PARTICLE TOUGHENING:

$$\Delta(K) \sim \left(C E' \sigma_y R f_v\right)^{1/2}$$



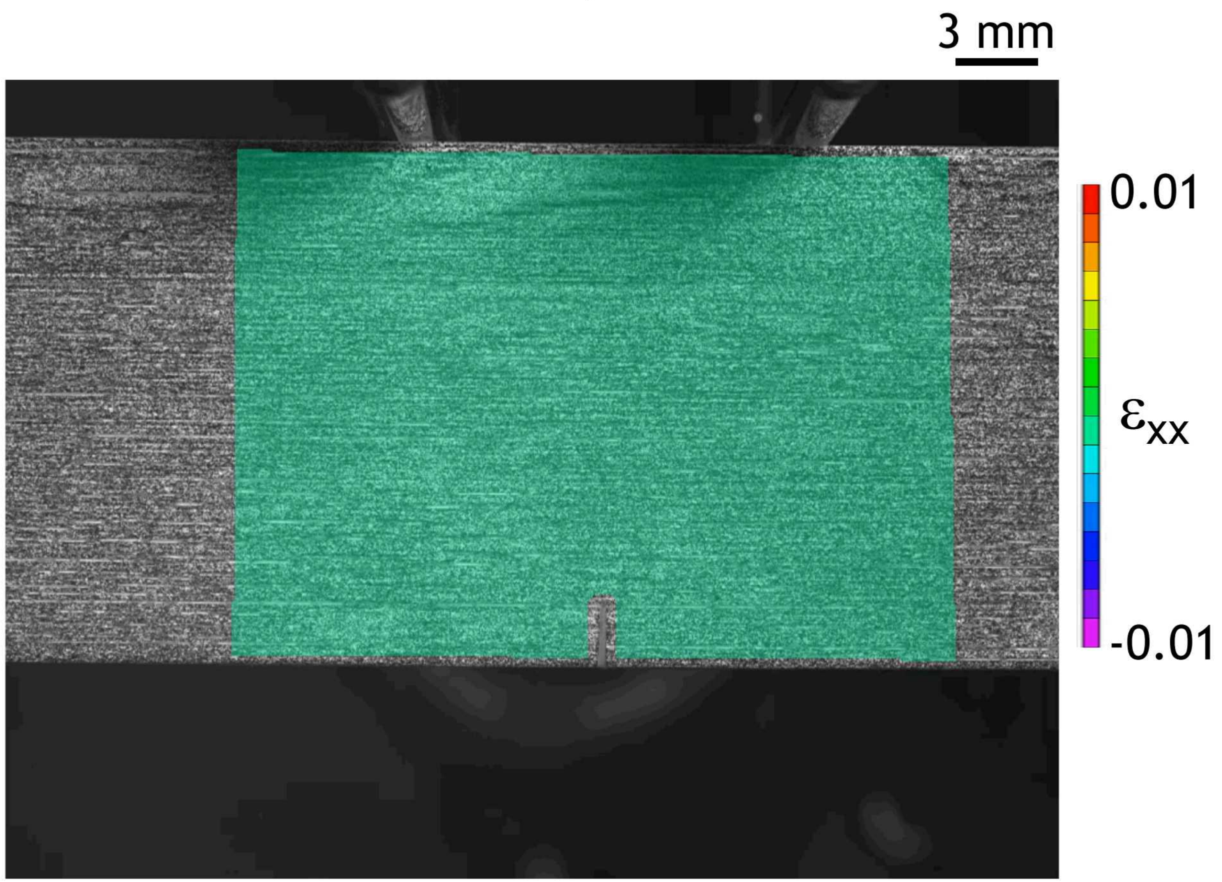
RO Ritchie, *Int. J. Fracture*, 1999

A simple proof of concept topology: Periodic array of cylindrical holes in an “arrestor” orientation

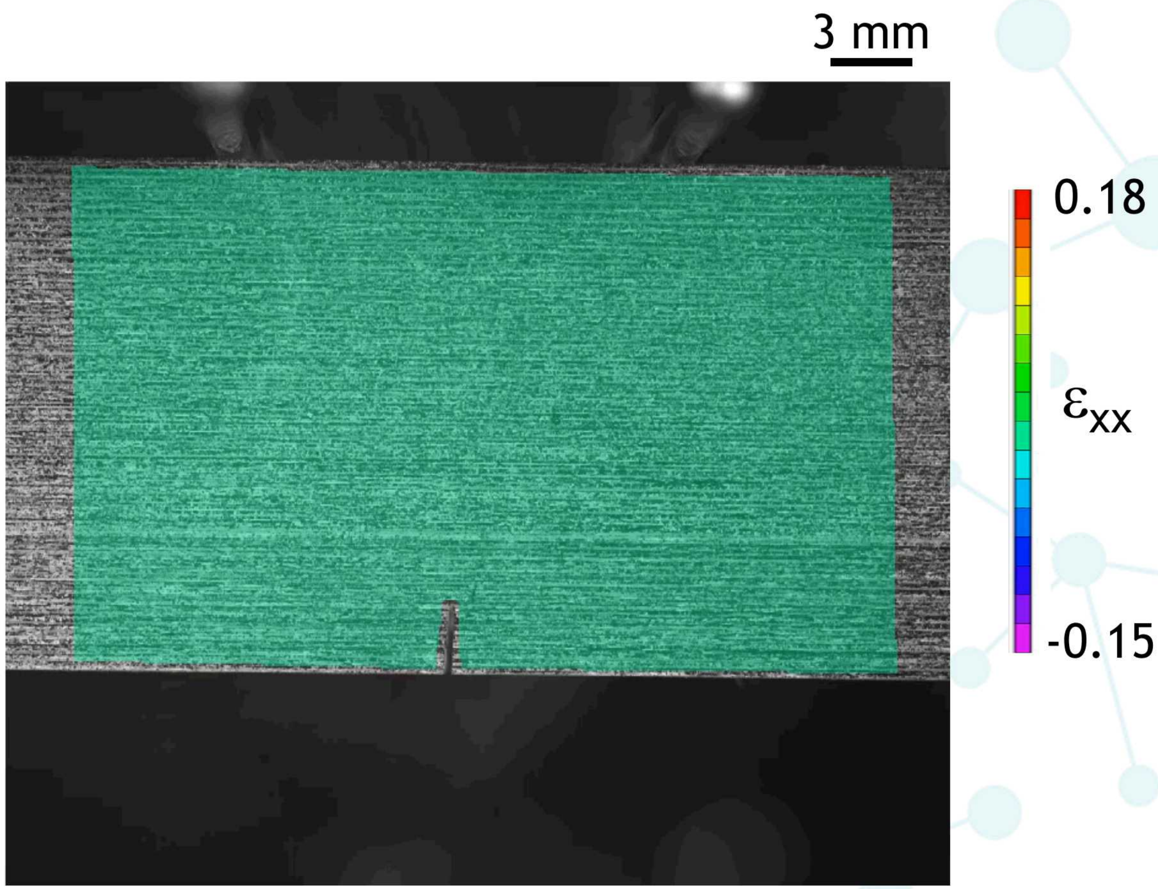


Limiting crack propagation in a brittle glassy polymer

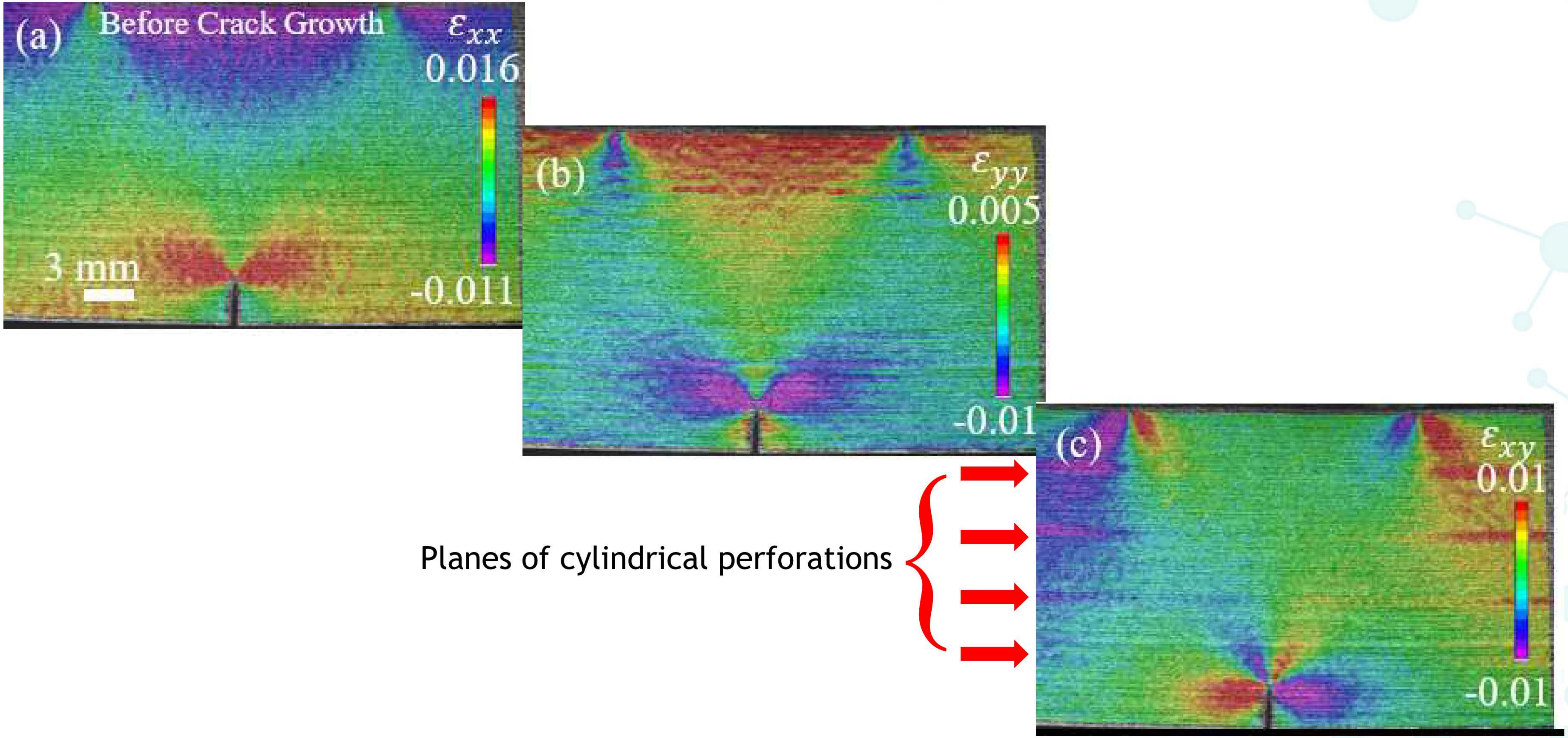
Unmodified



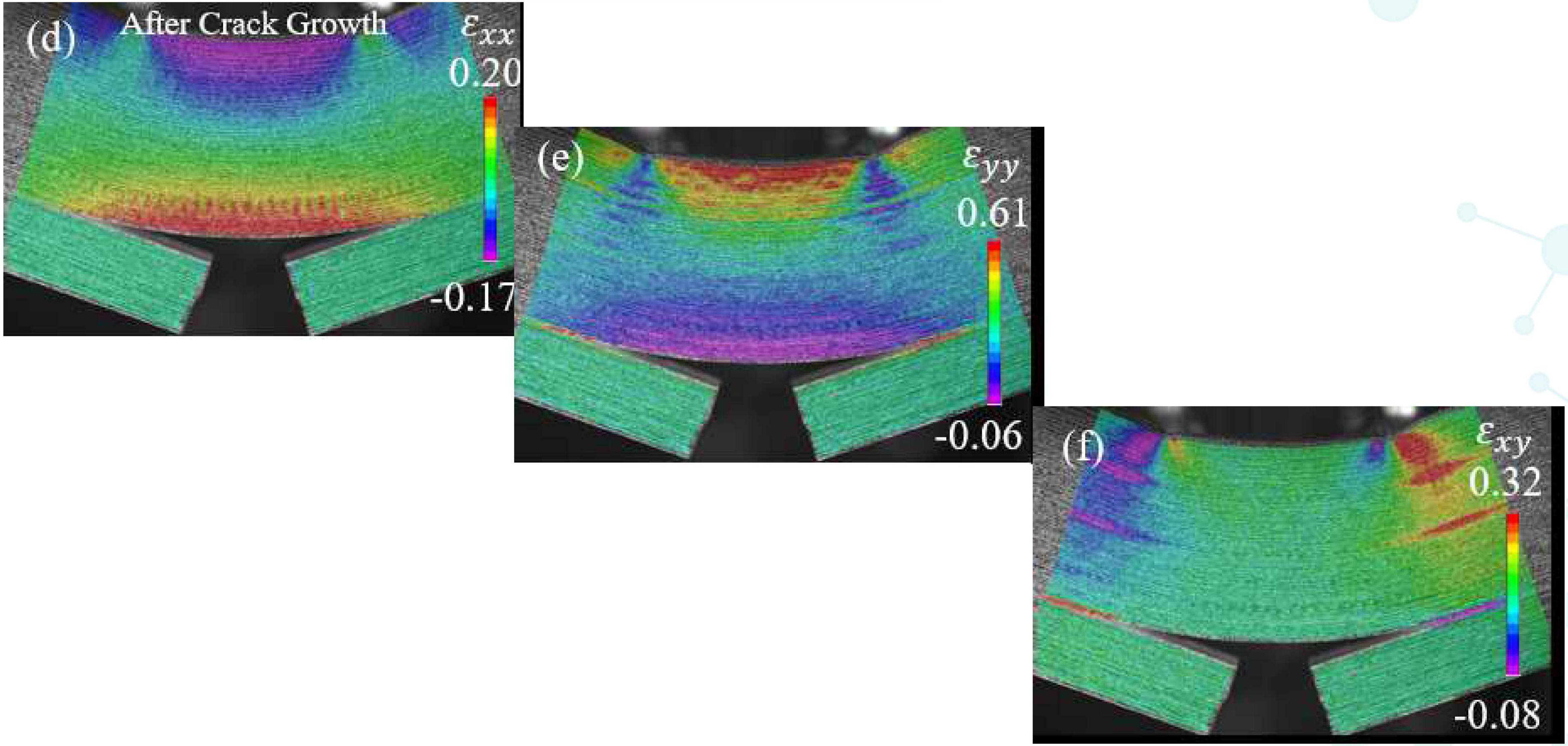
93% Dense… Four rows of cylindrical holes



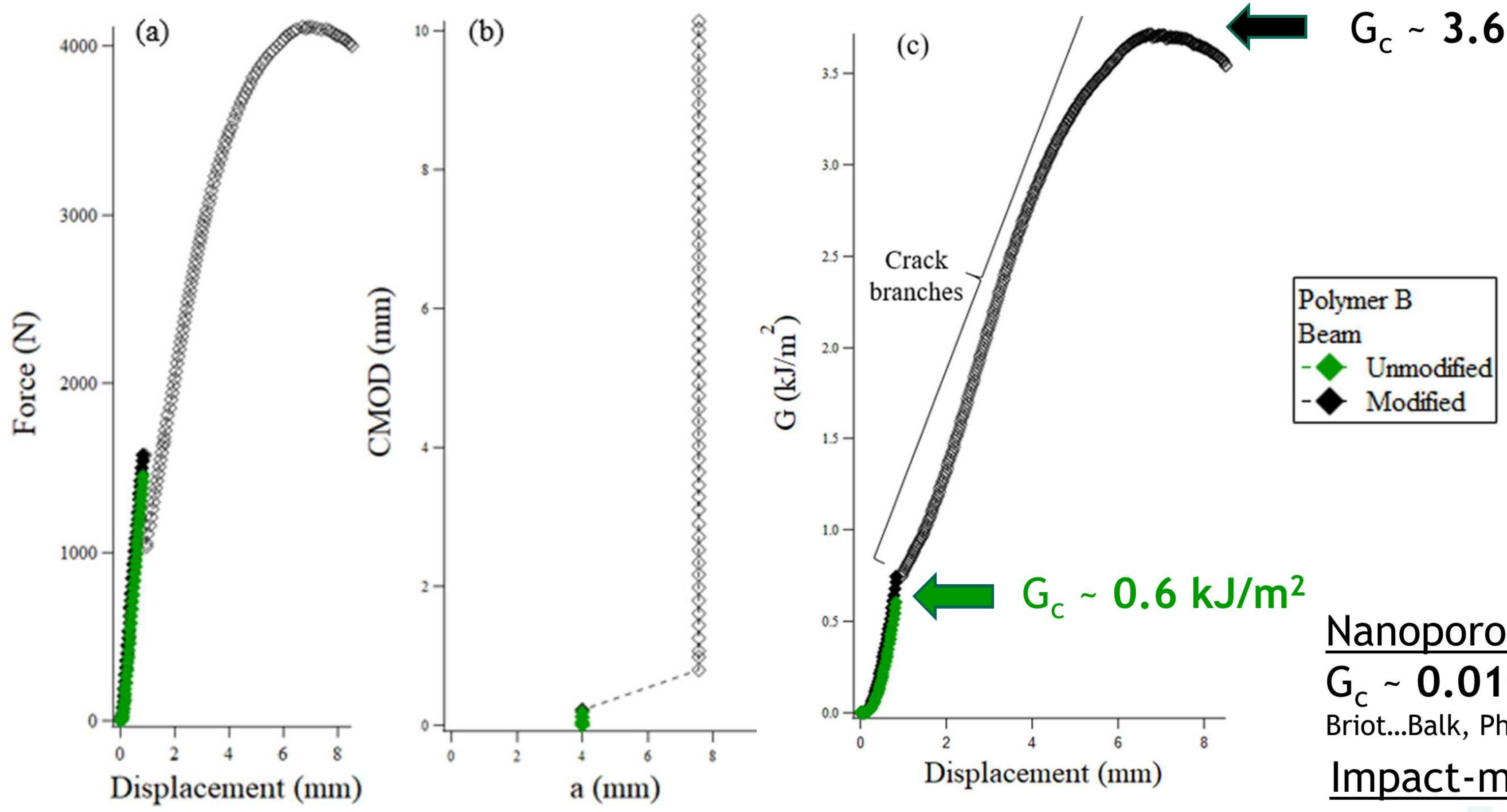
Material: Stratsys Durus, Polypropylene-like UV-Cured **Glassy Polymer**


(a)
Before Crack Growth
ε_{xx}
0.016
-0.011
3 mm
(b)
ε_{yy}
0.005
-0.01
(c)
ε_{xy}
0.01
-0.01
Planes of cylindrical perforations

Crack deflection, branching, pseudo-delamination along planes of cylindrical holes



600% improvement in fracture toughness over *base material* by adding air!



G_c ~ **3.6 kJ/m²**

G_c ~ **0.6 kJ/m²**

Nanoporous Gold,

G_c ~ **0.010 kJ/m²** density = 6.4 g/cm3

Briot…Balk, Phil Mag, 2014

Impact-modified Polypropylene

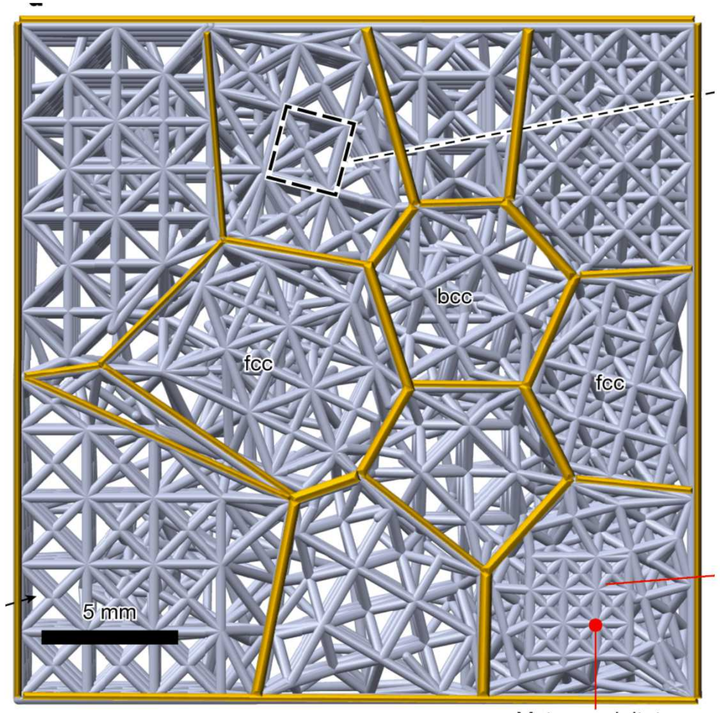
G_c =**2-5 kJ/m²**

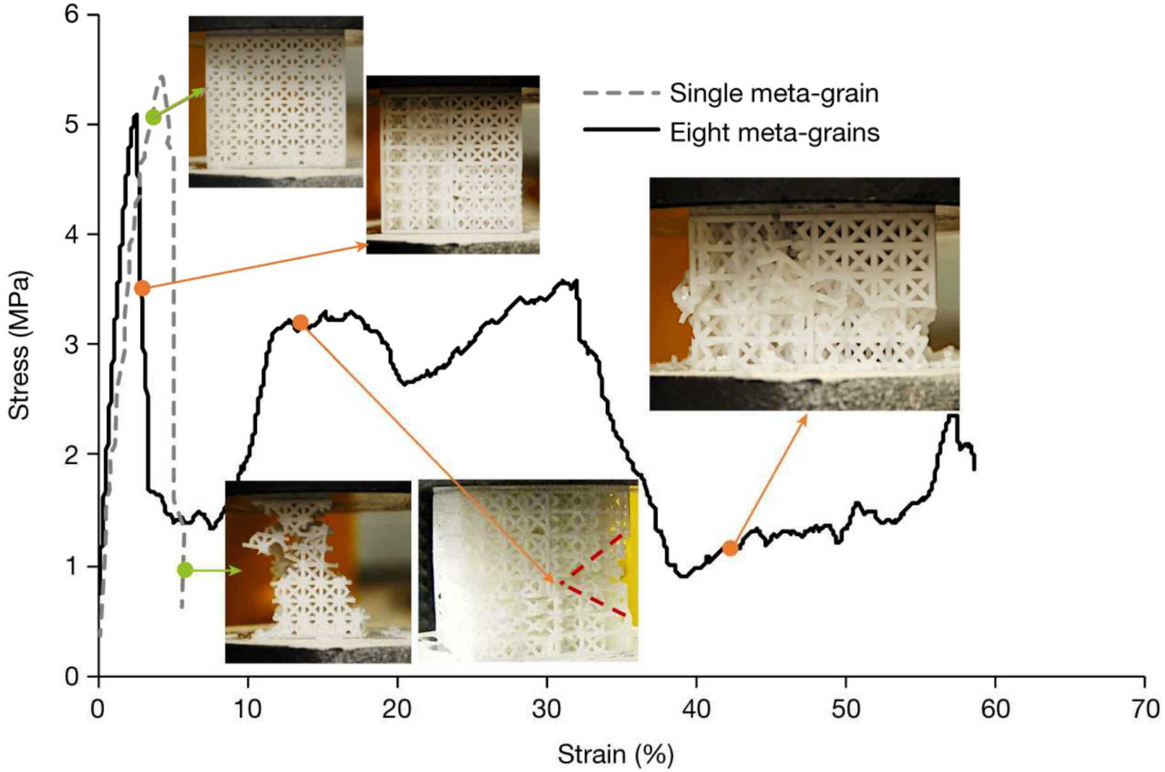
Li, Li, Tong, *Polymer Testing*, 1997

Conway, et al, *in preparation*

Are lattices tougher than foams?

Toughness vs Fracture Toughness



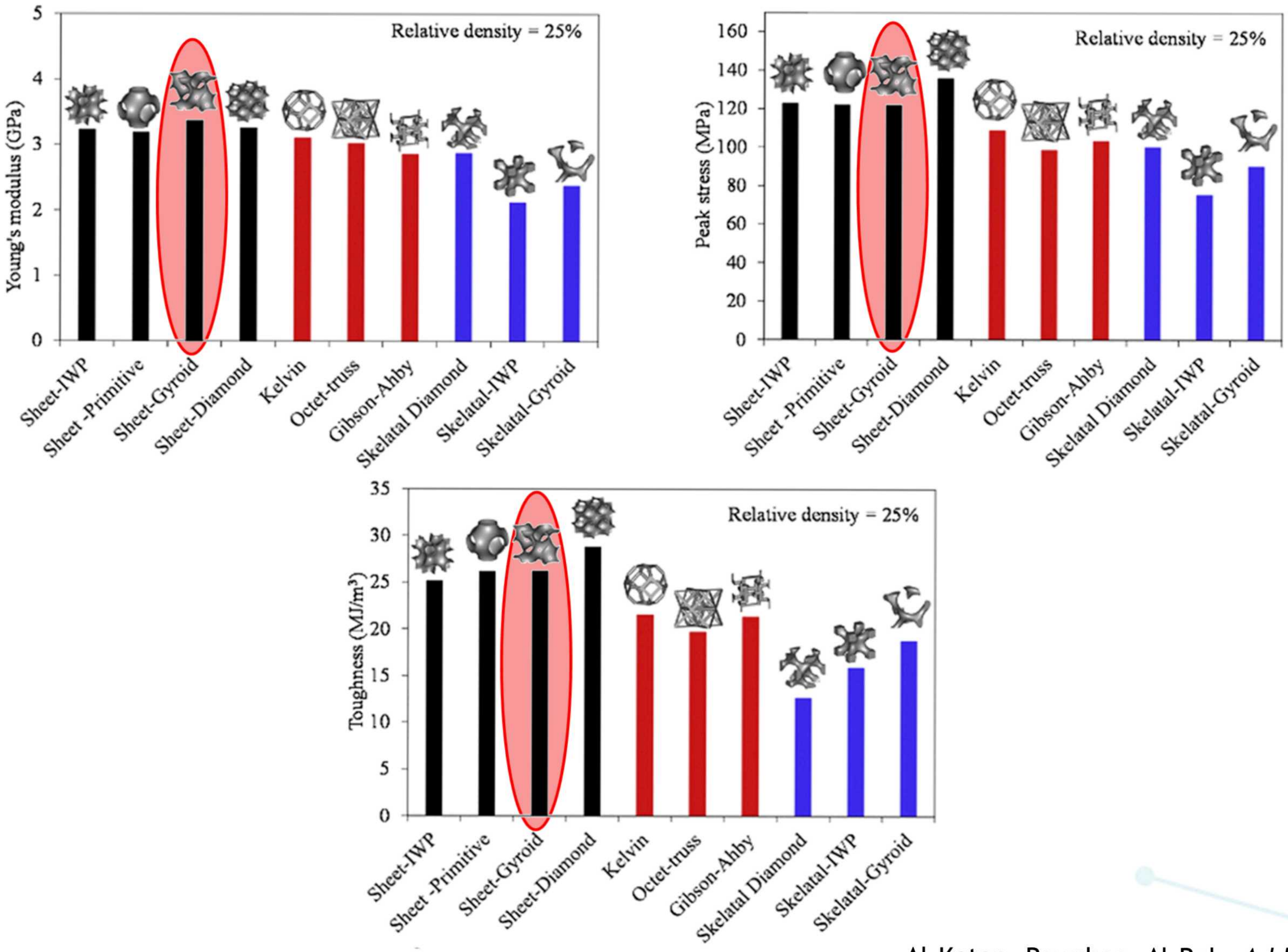


Pham, Liu, Todd, Lertthanasarn, **"Damage-tolerant architected materials inspired by crystal microstructure"**, *Nature*, 2019

The gyroid lattice: a triply periodic minimum surface

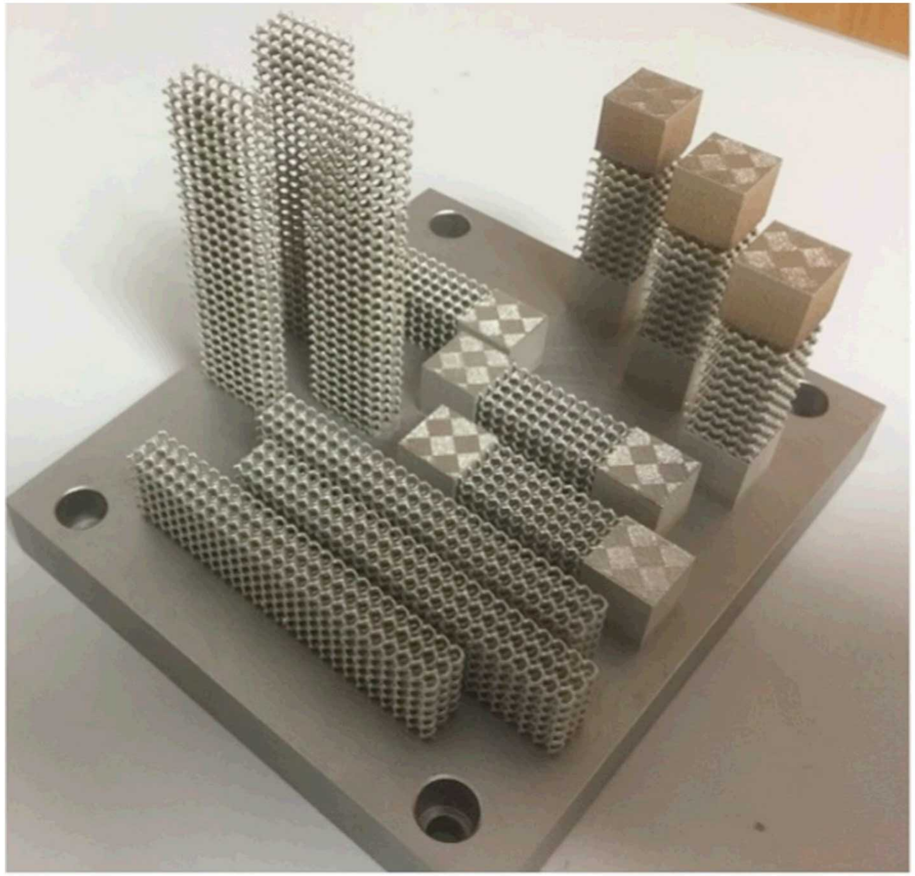
$$\sin x \cos y + \sin y \cos z + \sin z \cos x = 0$$

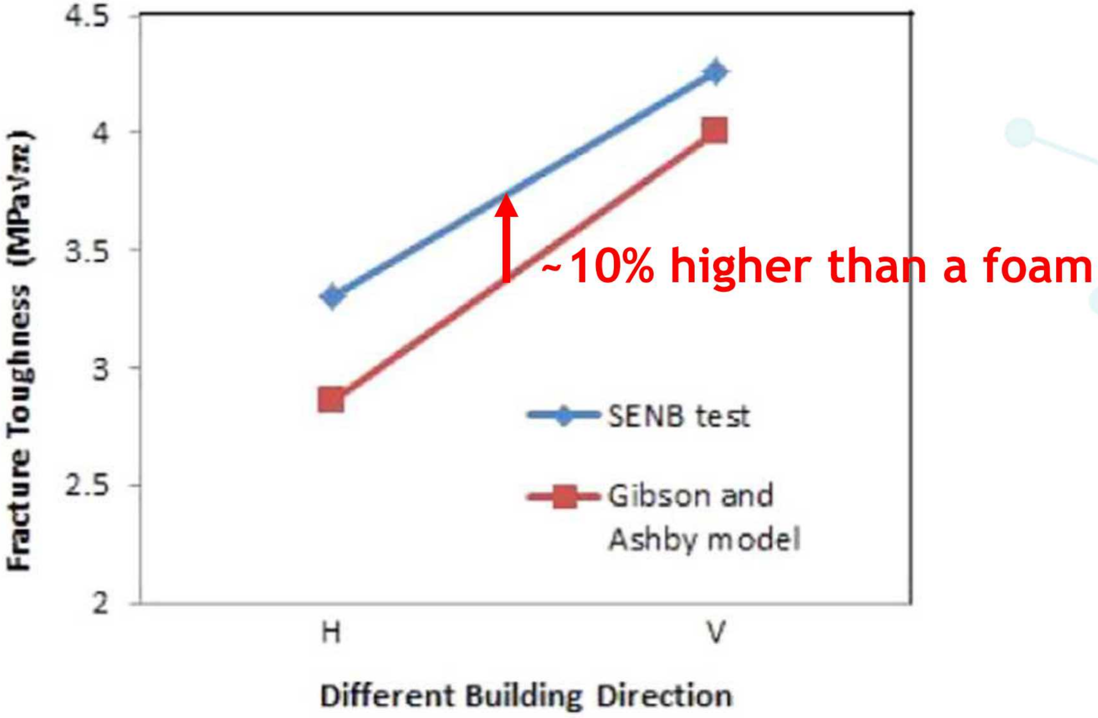
Why the gyroid?



Al-Ketan, Rowshan, Al-Rub, *Additive Manuf.*, 2018

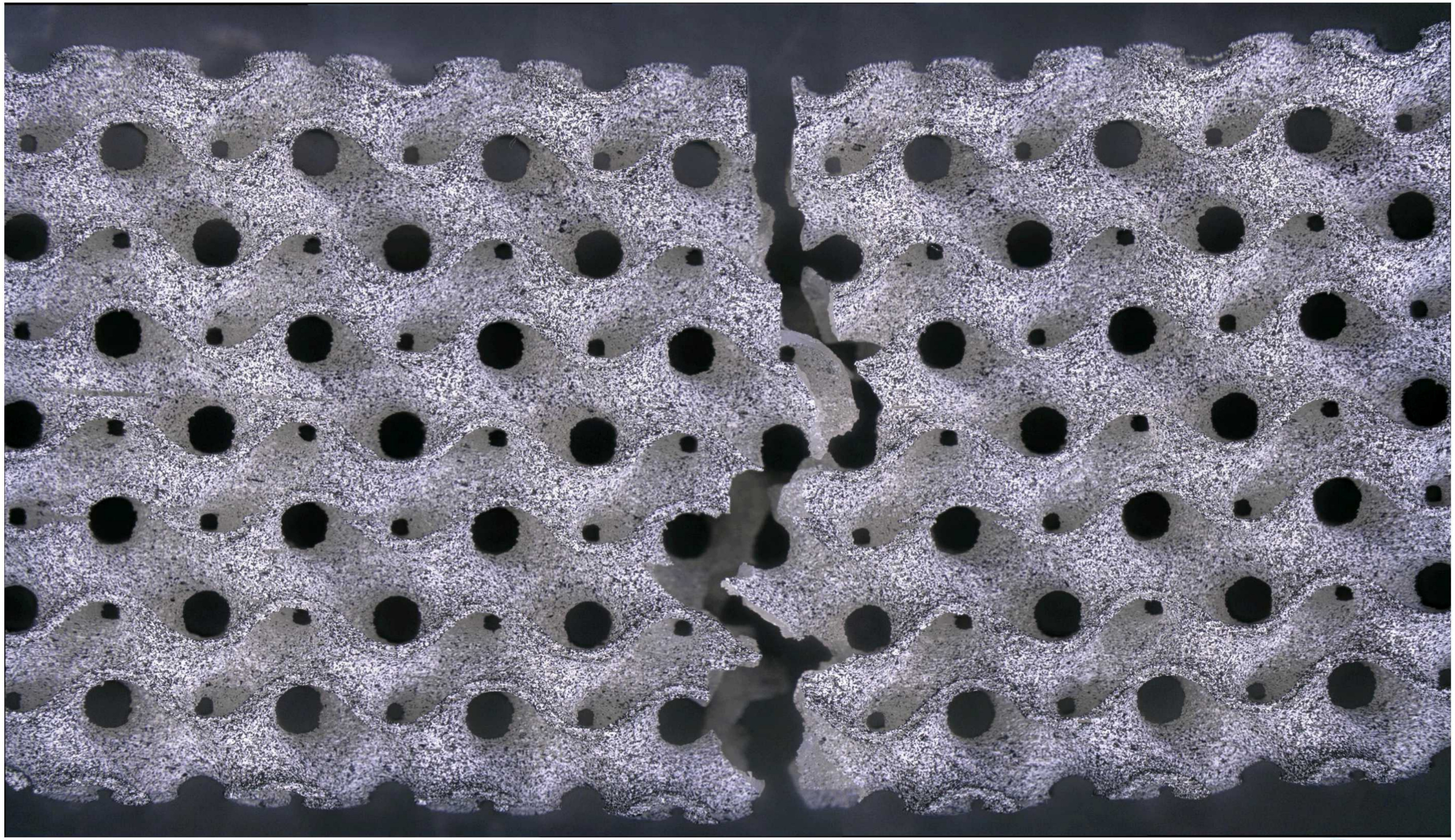
15% dense 316L gyroid





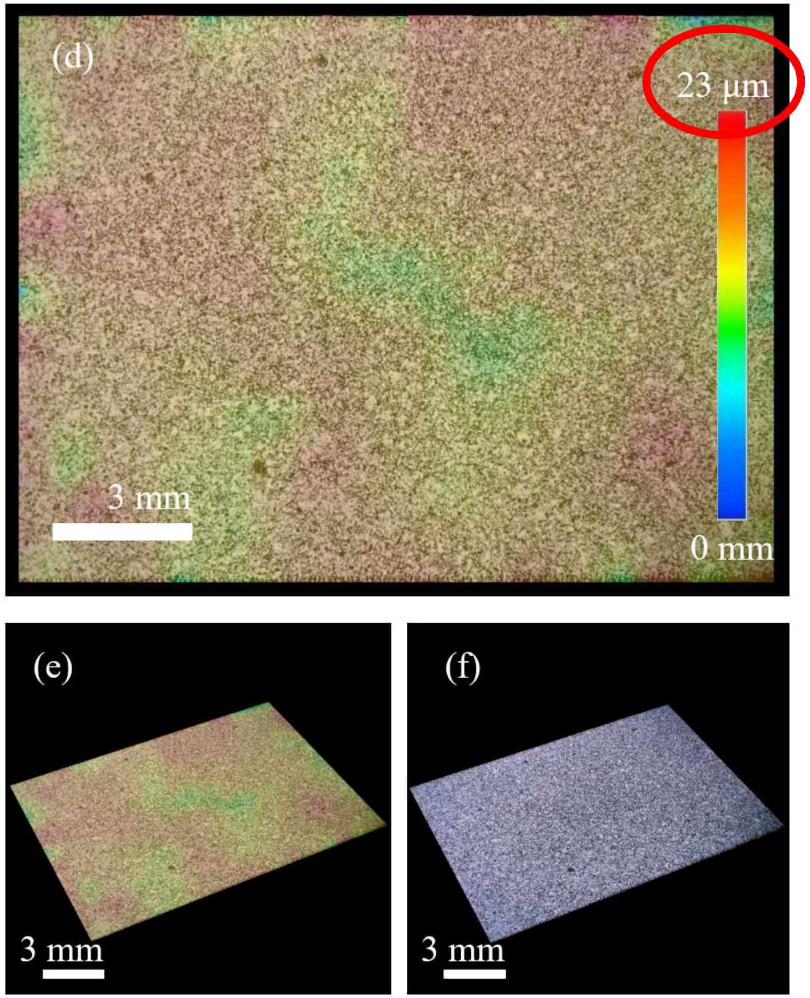
Alsalla, Hao, Smith, *Mater Sci Eng A*, 2016

Crack deflection…

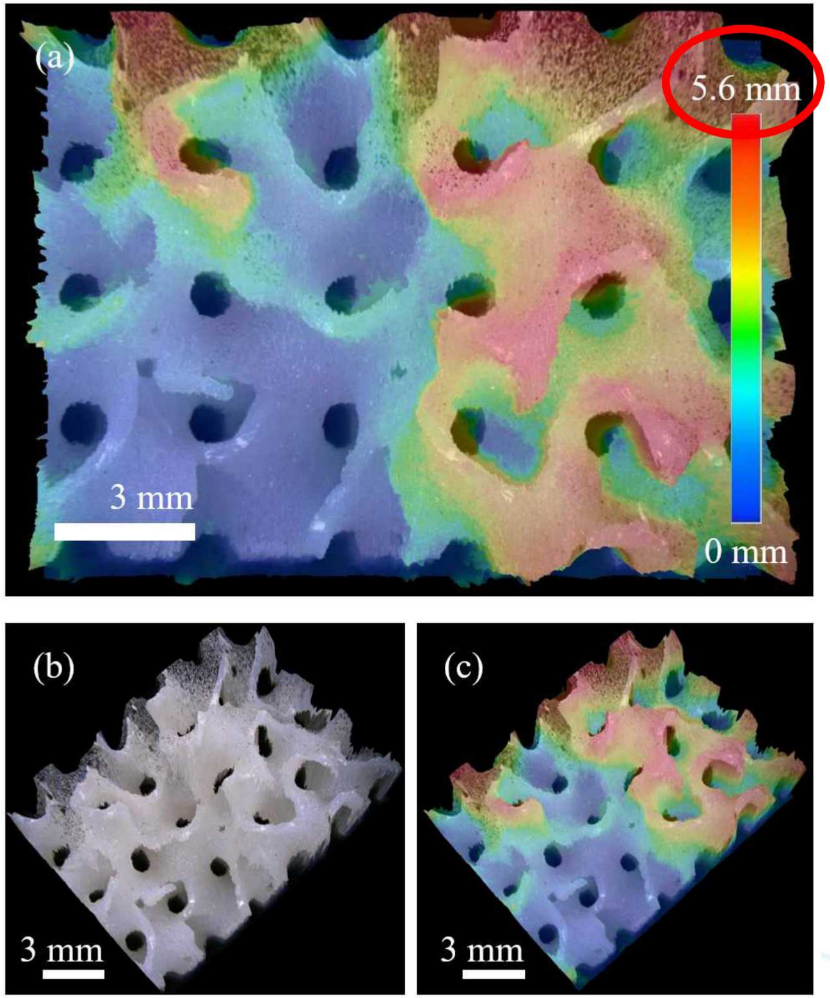


The Gyroid architecture toughens by crack deflection…

Fracture surface of solid material:
brittle UV-cured polymer, Verowhite

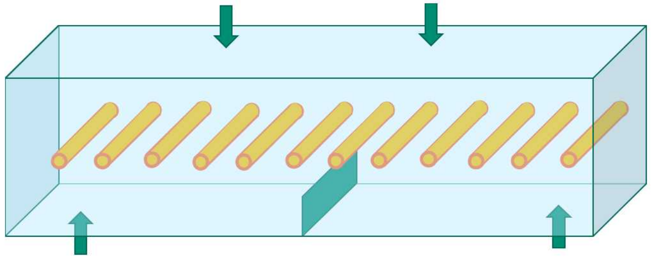


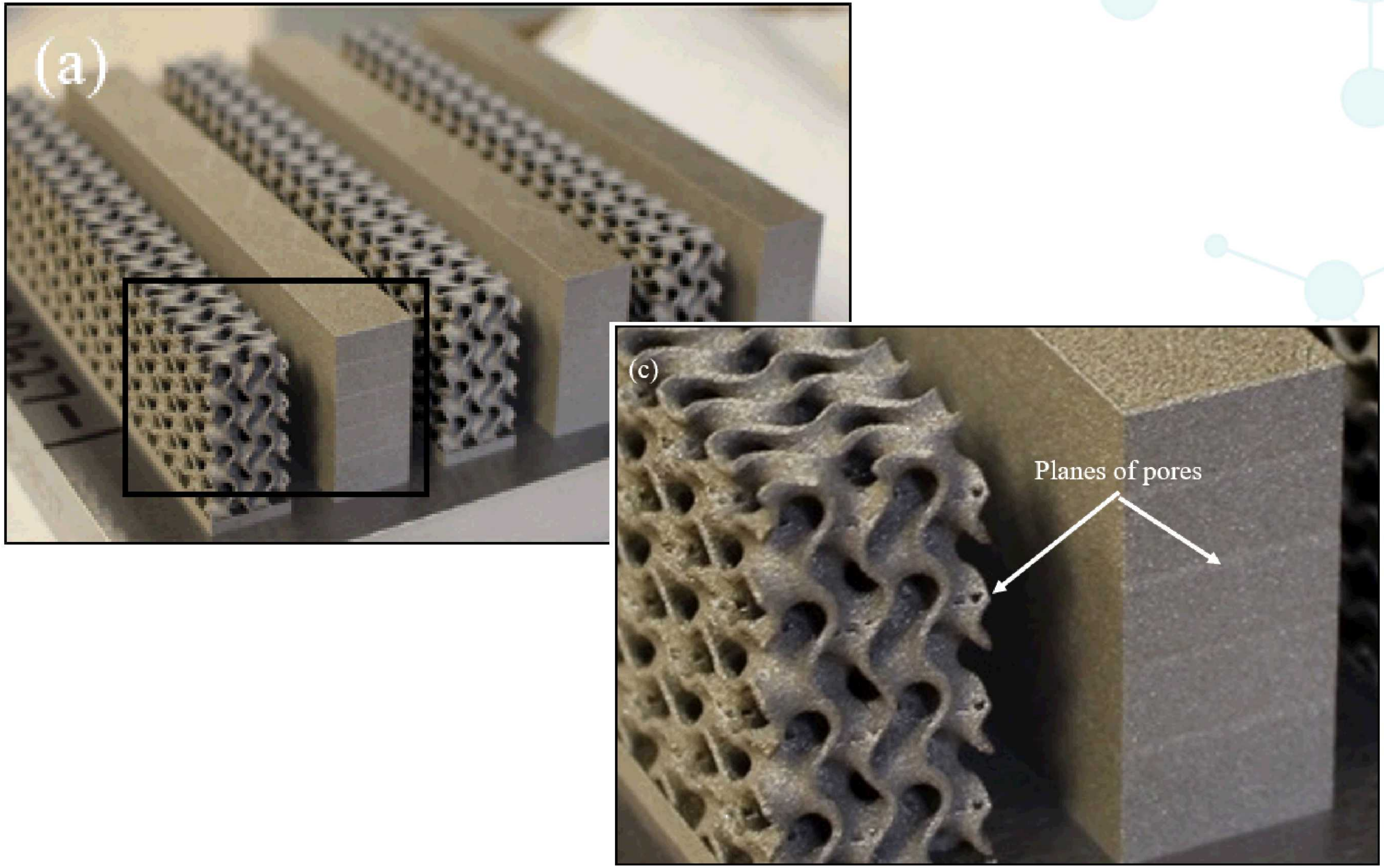
Fracture surface of gyroid architecture:
same brittle polymer, Verowhite



Conway, et al, *in preparation*

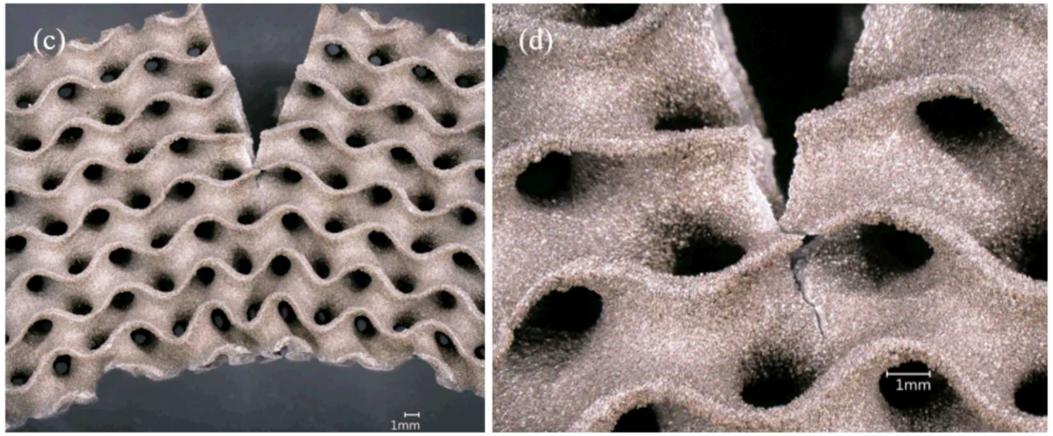
Can we further toughen a gyroid by adding hierarchical porosity?



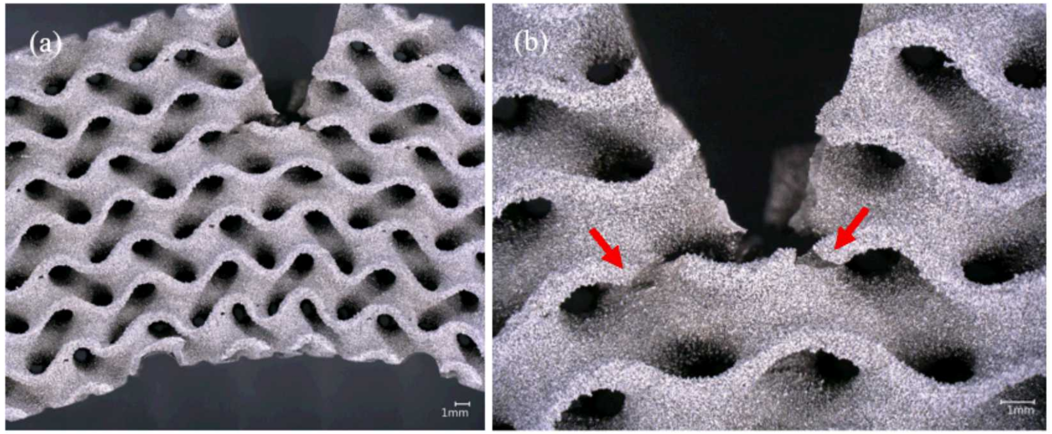


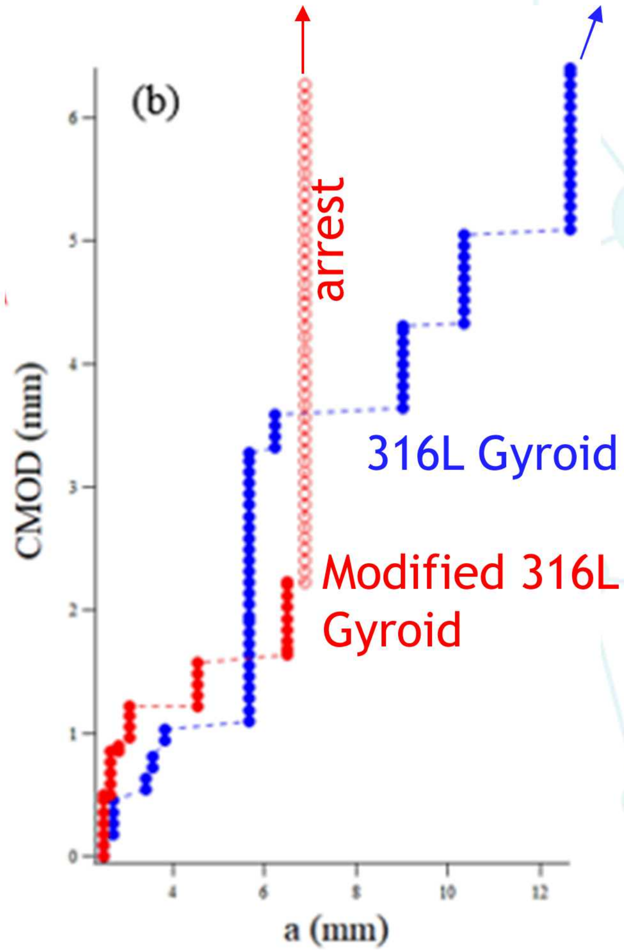
Crack deflection by additional porosity

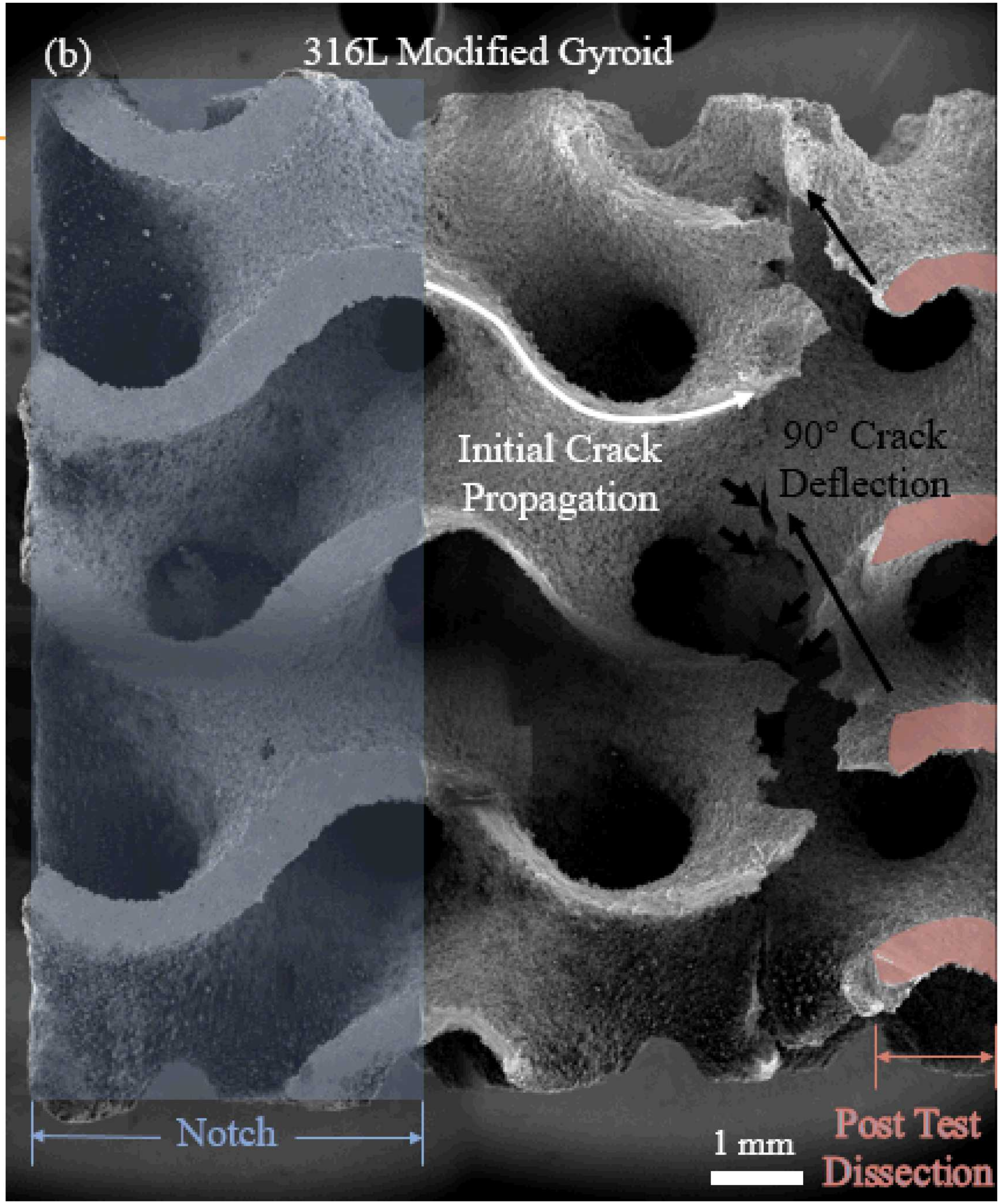
Unmodified gyroid, 316L



Gyroid with additional cylindrical pores, 316L






(b)
316L Modified Gyroid
Initial Crack Propagation
90° Crack Deflection
Notch
1 mm
Post Test Dissection

Additive manufacturing enables generative design…

3Dprint.com

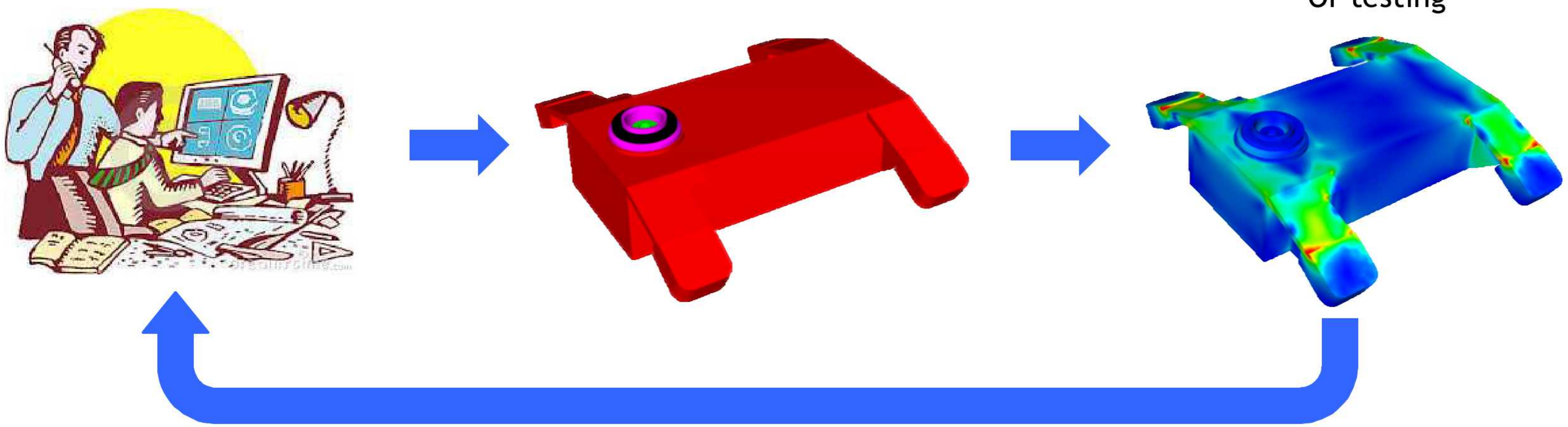
Topology optimization, a form of generative design

CURRENT

specify form

design

verify function
w/FEA
Or testing

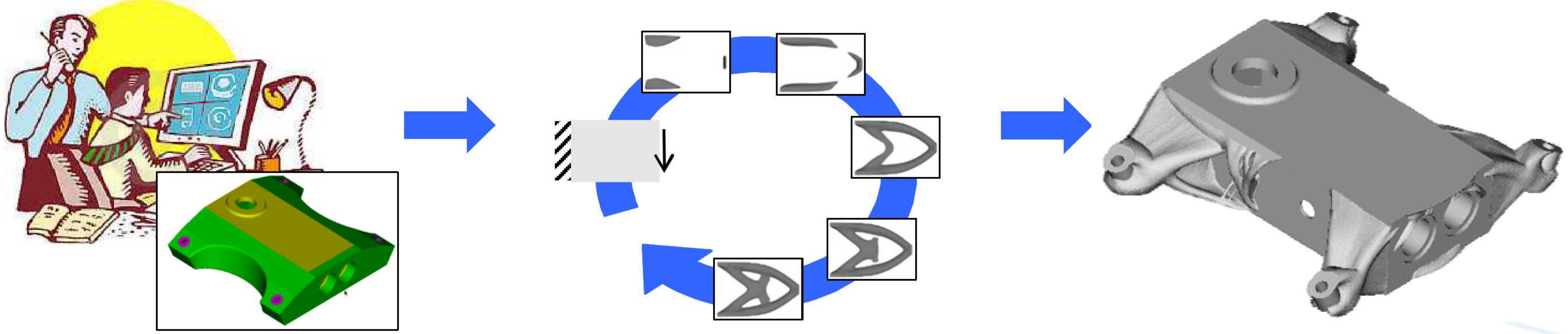


NEW

specify design domain
& function

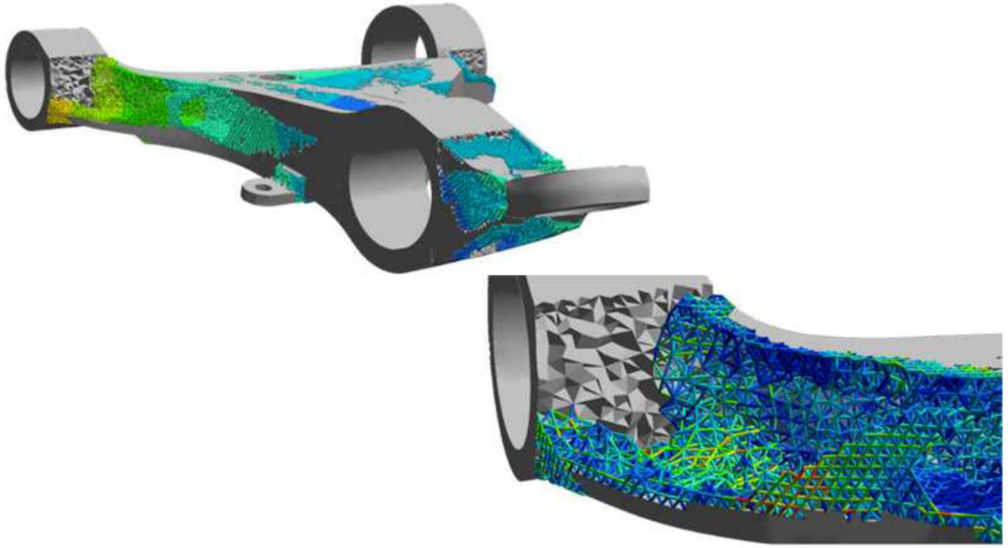
use topology optimization to determine form
that meets function

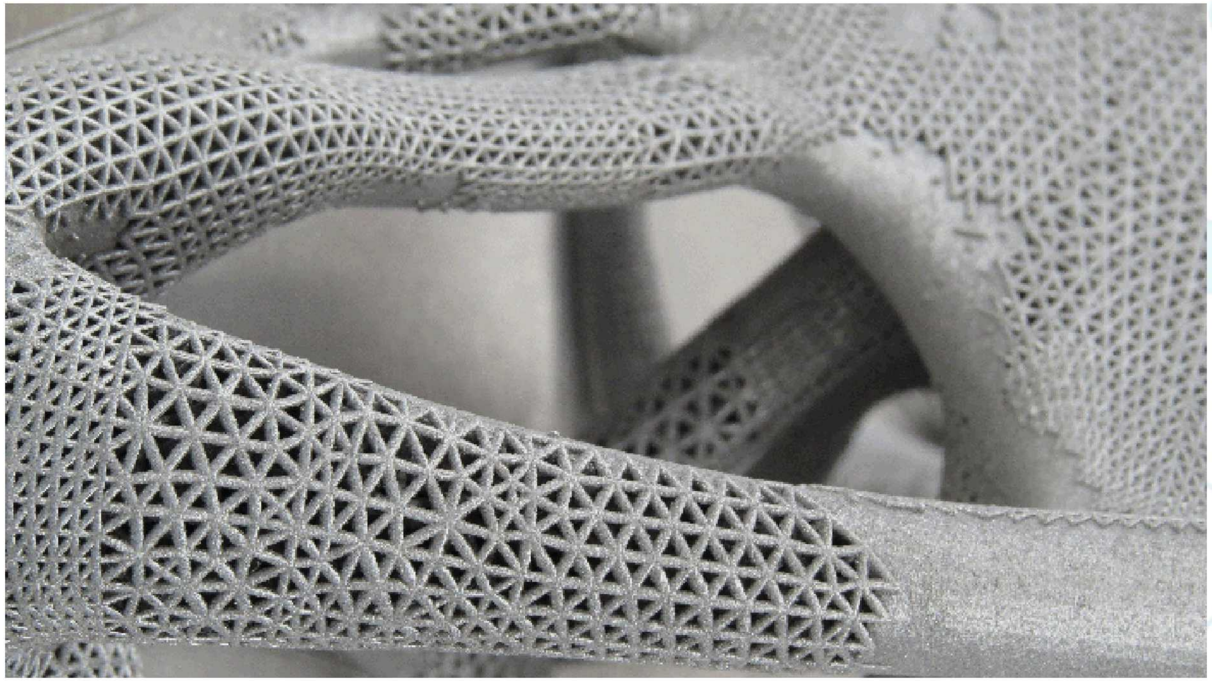
optimized
design form



Galjaard, Hofman and Ren,
Biomimetic Lightweight…, 2015

Two-scale topology optimization for fracture resistance?

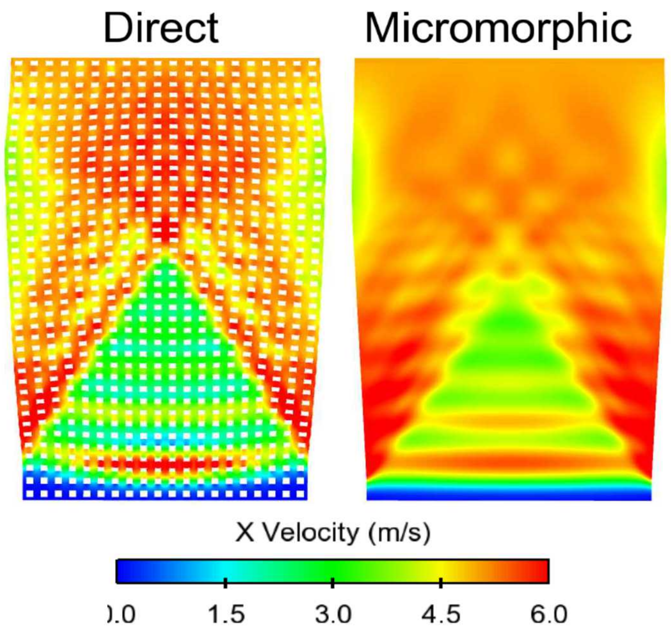




Examples: nTopology, Altair hyperworks

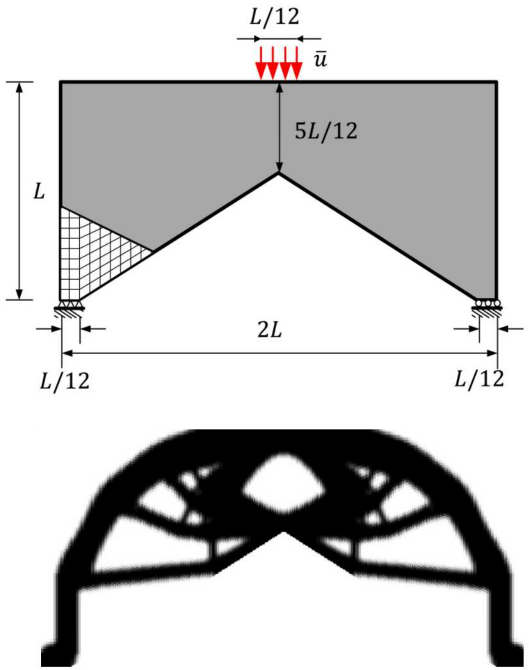
Three challenges for optimized design of fracture resistance

1. For computational tractability, you must employ **homogenization**



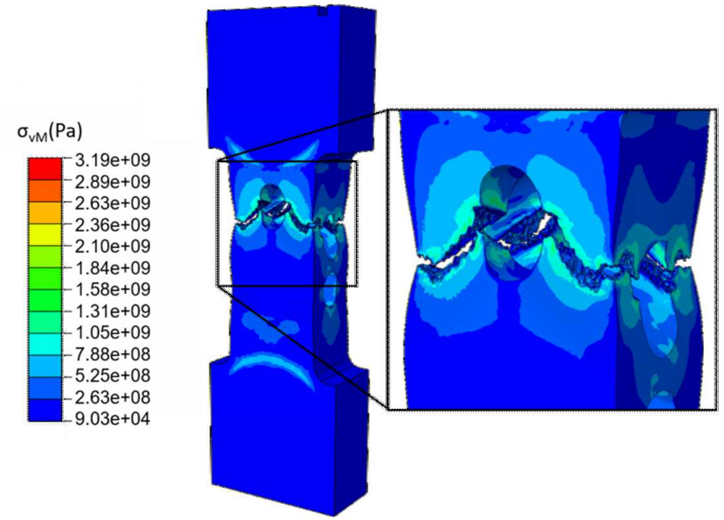
Dingreville, Robbins, Voth, *JOM*, 2013

2. **Nonlinear** elastoplastic response is path dependent: challenging for optimization



Alberdi, Zhang, Khandelwal, *Numerical Methods in Eng.*, 2018

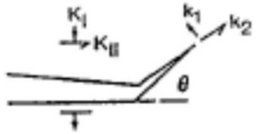
3. Predicting **ductile rupture** in FEA is challenging



Kramer…Boyce, *Int. J. Fracture*, 2019

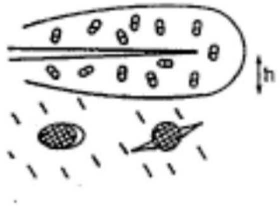
Extrinsic toughening mechanisms for brittle materials

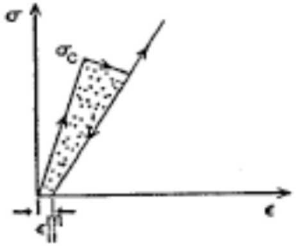
- CRACK DEFLECTION



- MICROCRACK TOUGHENING:

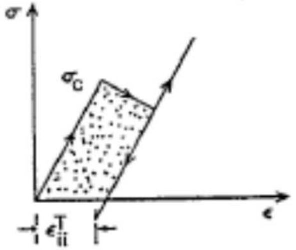
$$\Delta(K) \sim E' f_v \varepsilon_{ii}^{m} \sqrt{h}$$





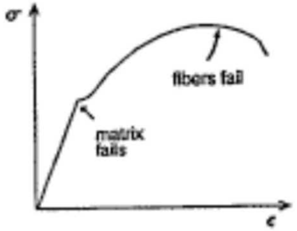
- TRANSFORMATION TOUGHENING:

$$\Delta(K) \sim E' f_v \varepsilon_{ii}^{T} \sqrt{h}$$



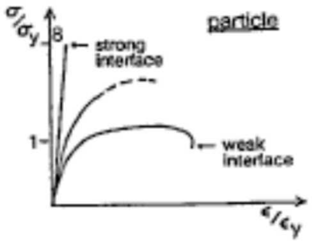
- BRITTLE FIBER/WHISKER TOUGHENING:
  (crack bridging)

$$\Delta(K) \sim \left(2 f_v E' \tau_i \ell^2 / \alpha\right)^{1/2}$$



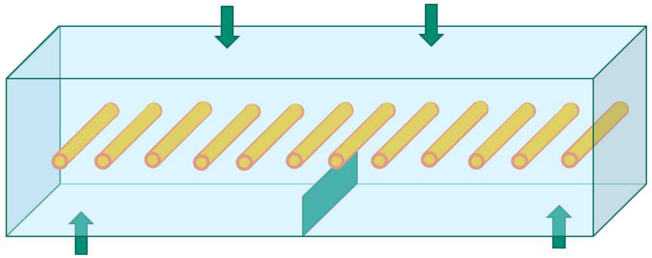
- DUCTILE PARTICLE TOUGHENING:

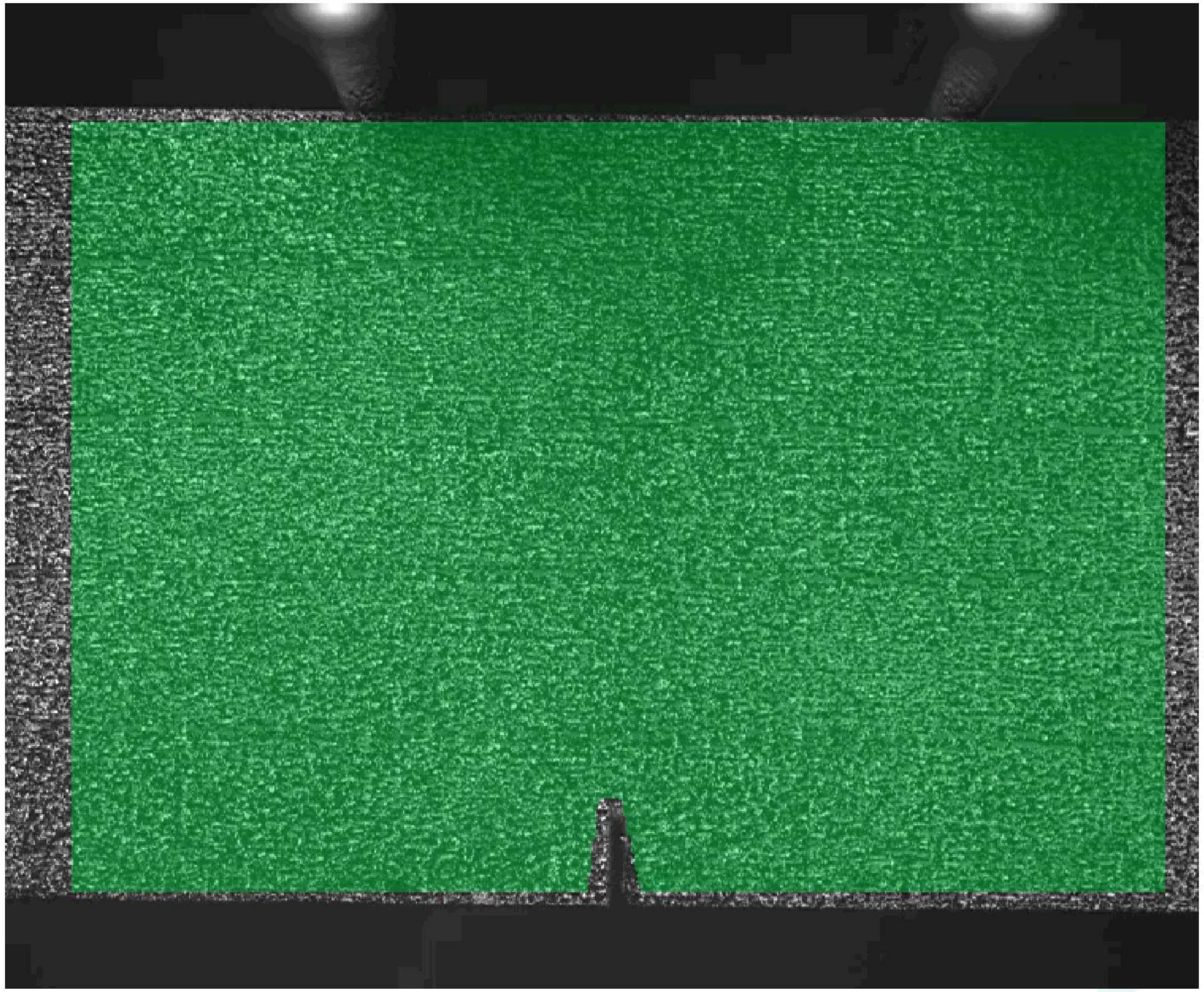
$$\Delta(K) \sim \left(C E' \sigma_y R f_v\right)^{1/2}$$



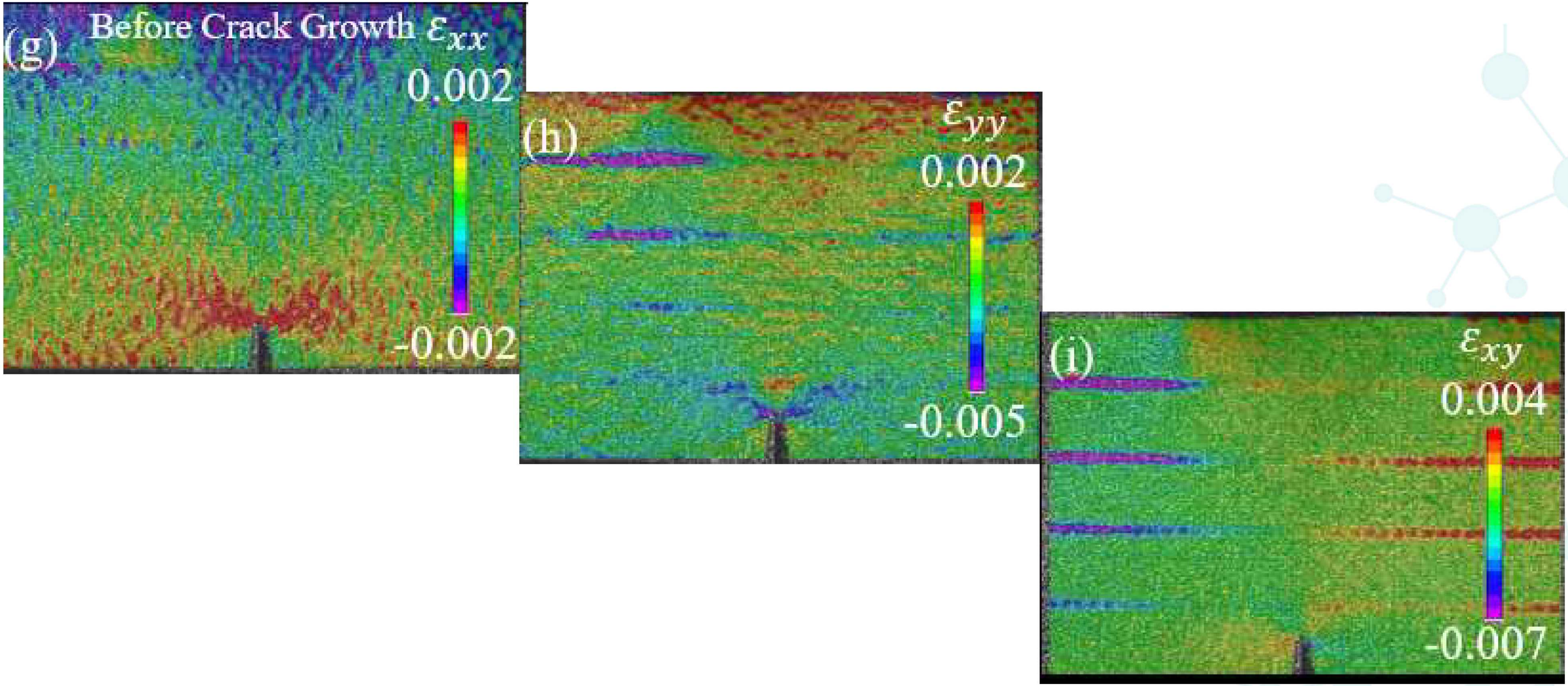
RO Ritchie, *Int. J. Fracture*, 1999

Another form of toughening: pseudo-blunting

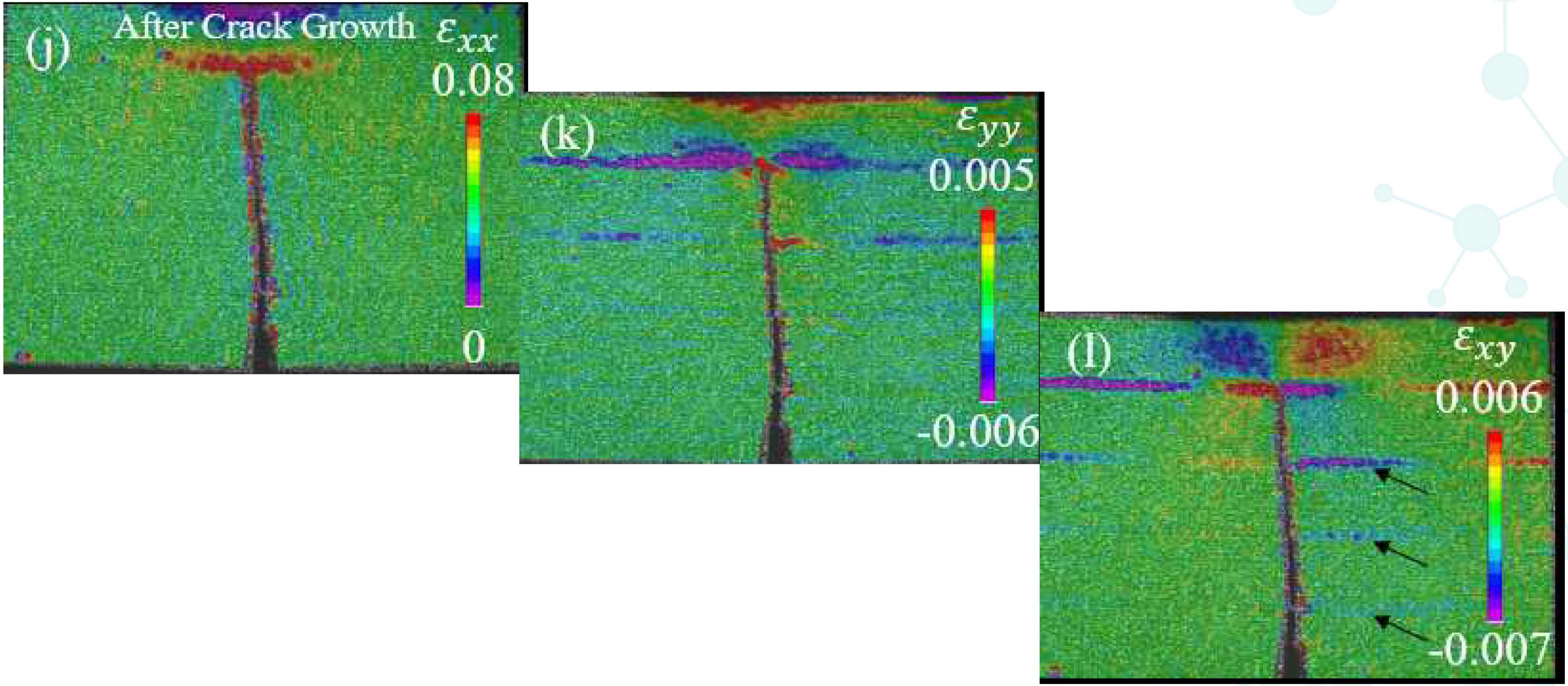




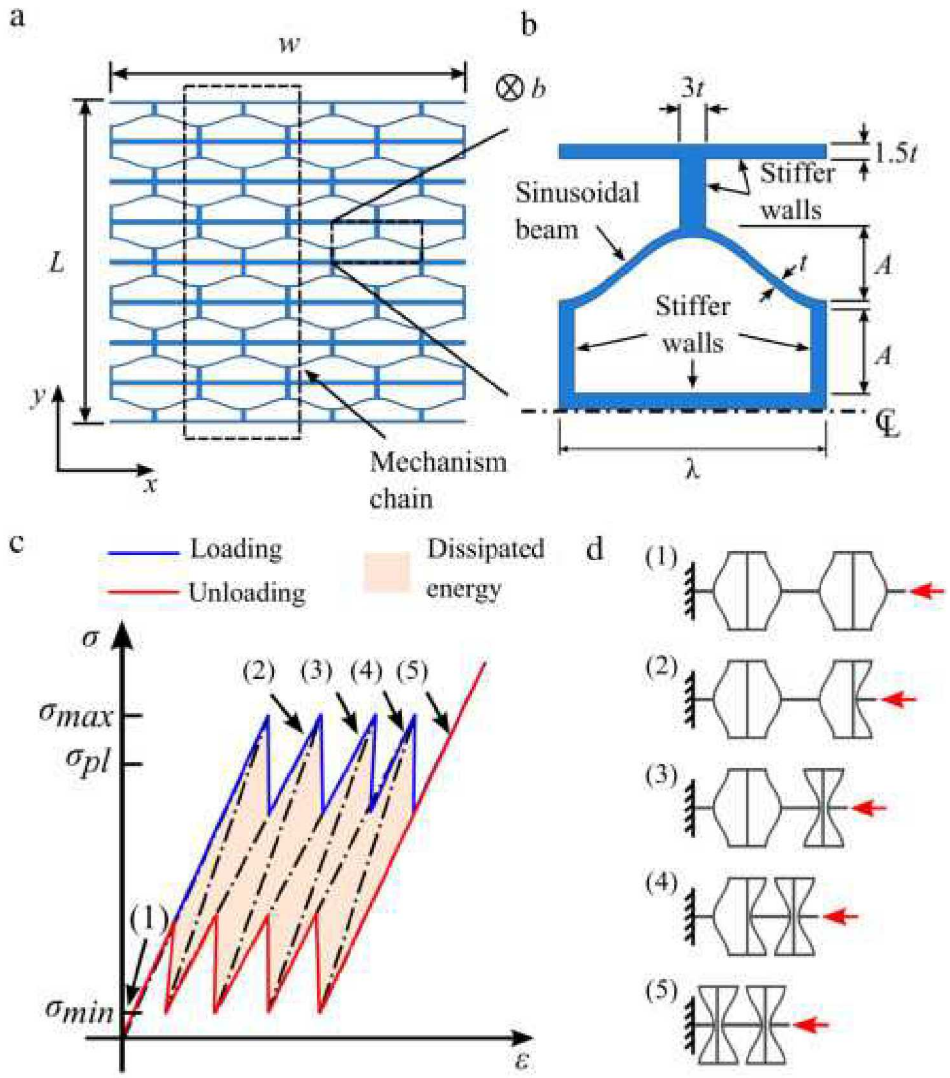
A second form of toughening: pseudo-blunting

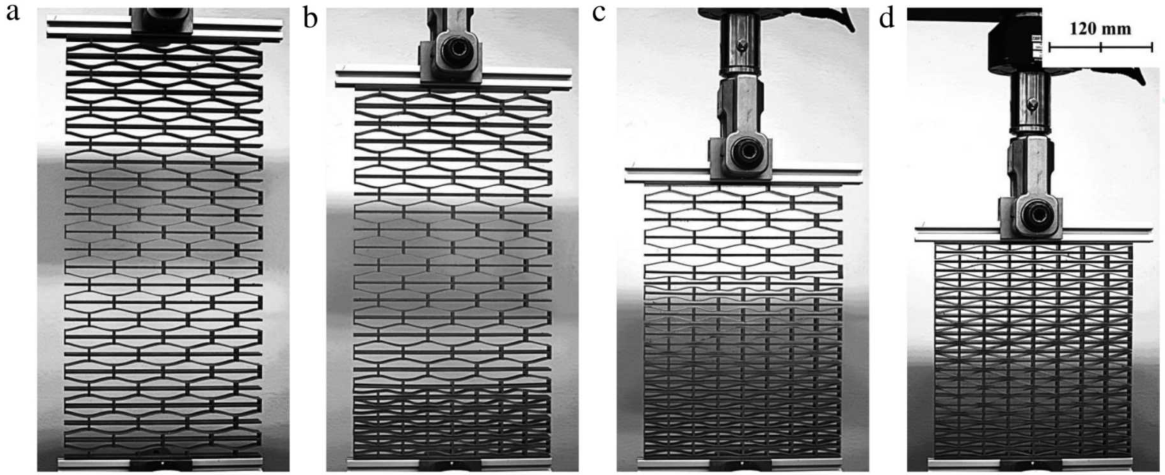


A second form of toughening: pseudo-blunting



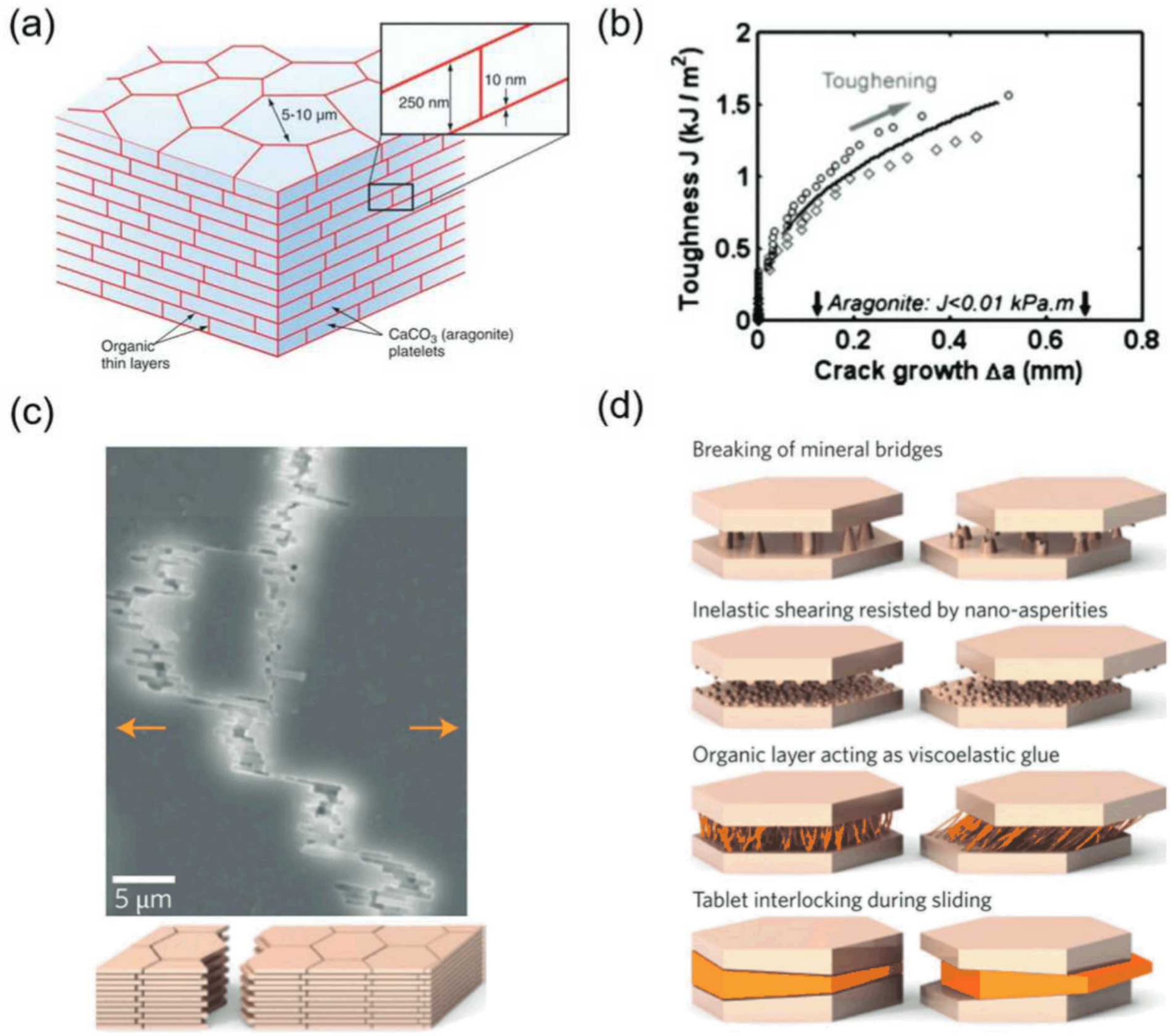
Any material can be a phase transforming material!





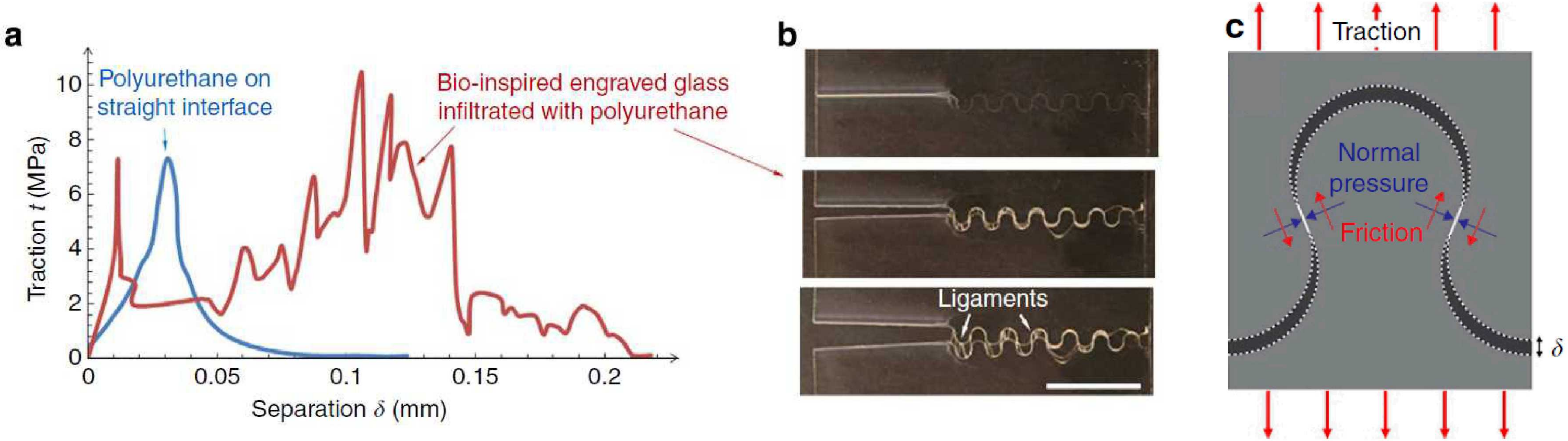
Restrepo, Mankame, Zavattieri, *Extreme Mechanics Letters*, 2015

Localized shearing for toughening



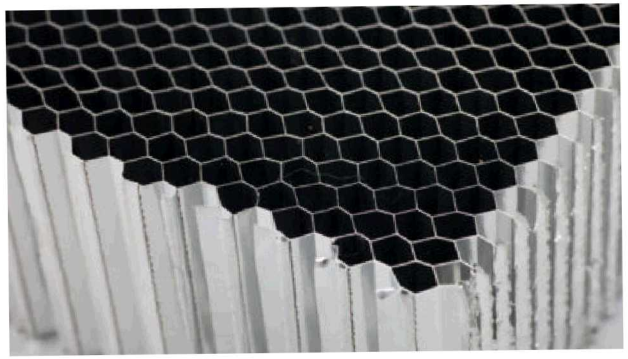
Huang…Ritchie…Kisailus, *Advanced Materials*, 2019

Etching a crack path on a brittle material…

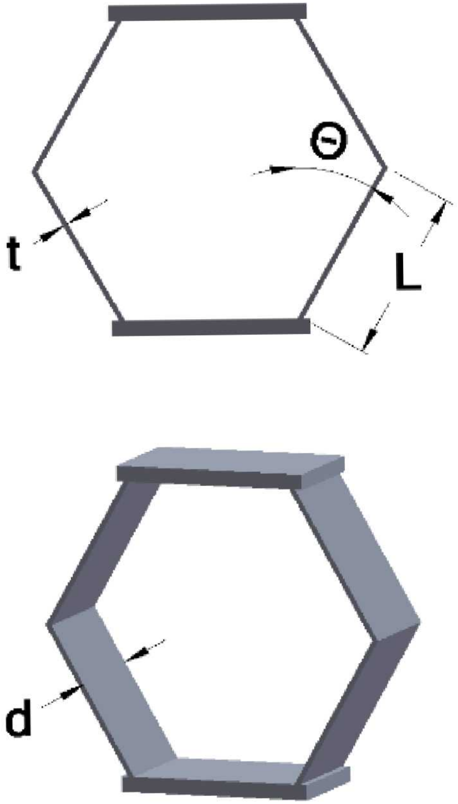


Mirkhalaf, Khayer Dastjerdi, Barthelat, *Nature Comm*, 2014

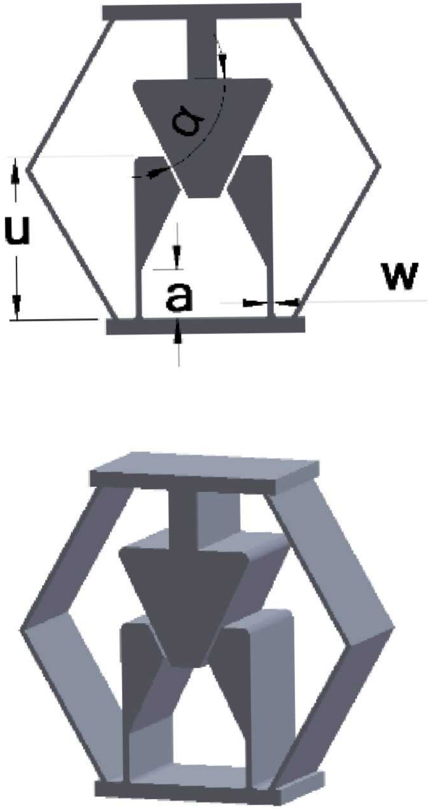
Adding friction to the honeycomb topology…



honeycomb

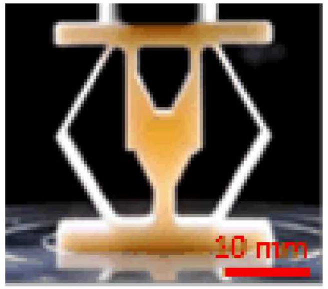


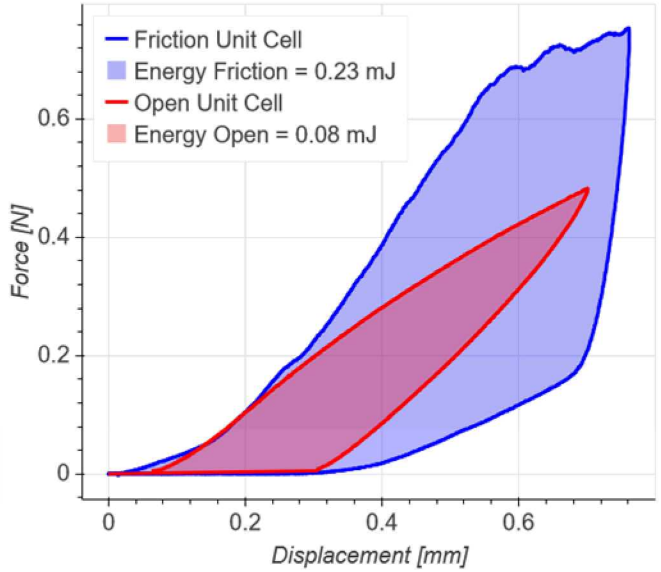
honeycomb with
friction elements



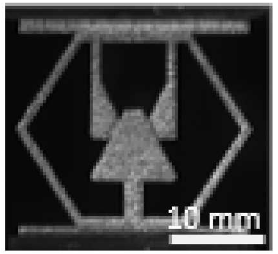
Architected energy dissipation

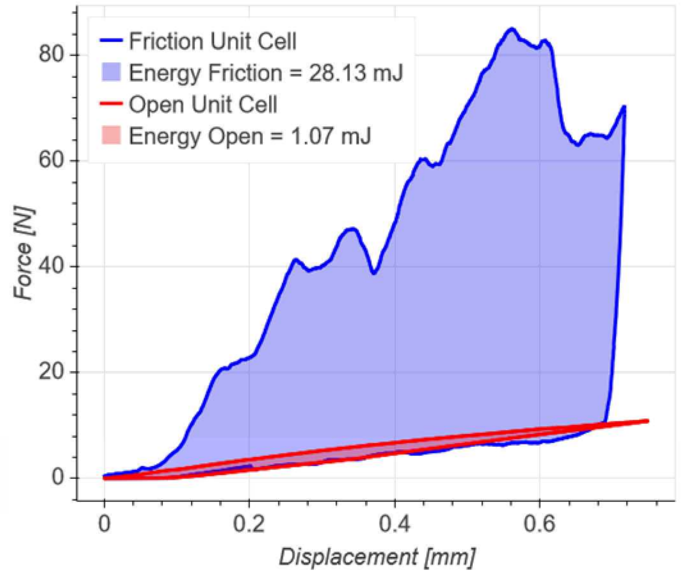
In a polymer



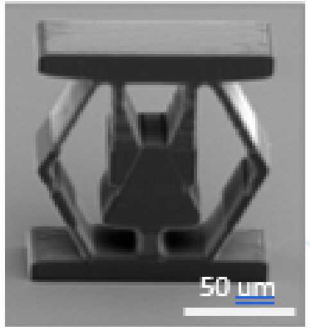


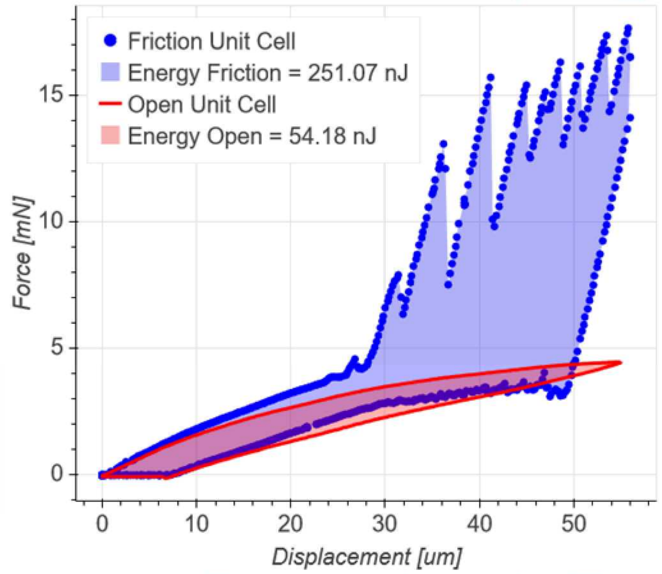
In a metal



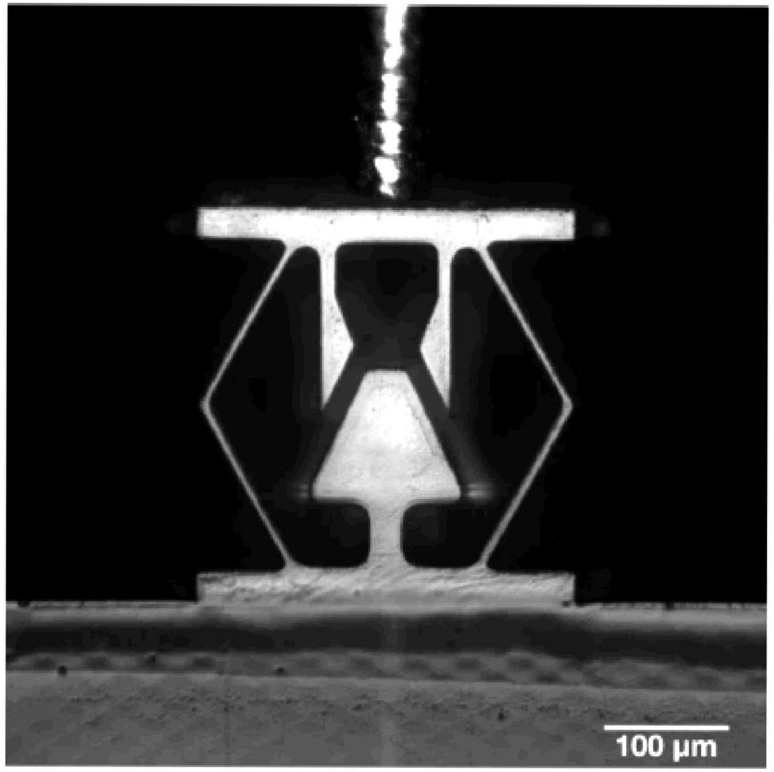


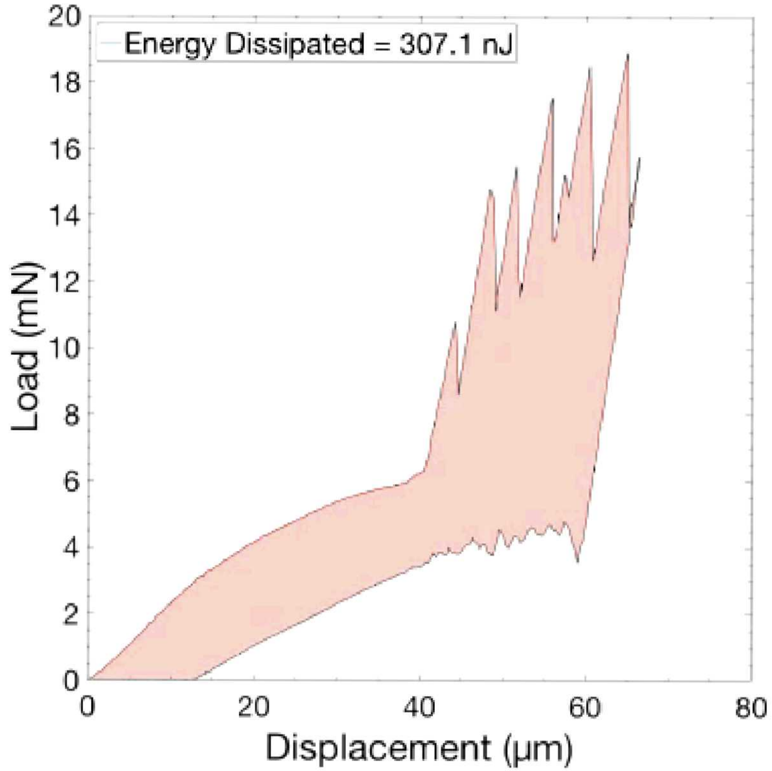
At the microscale



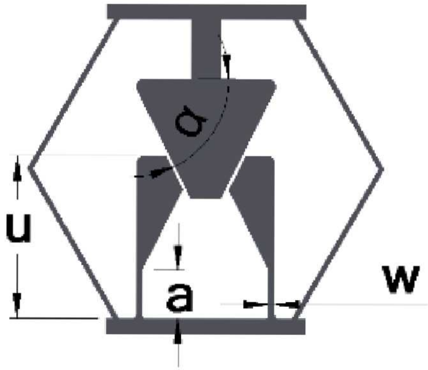


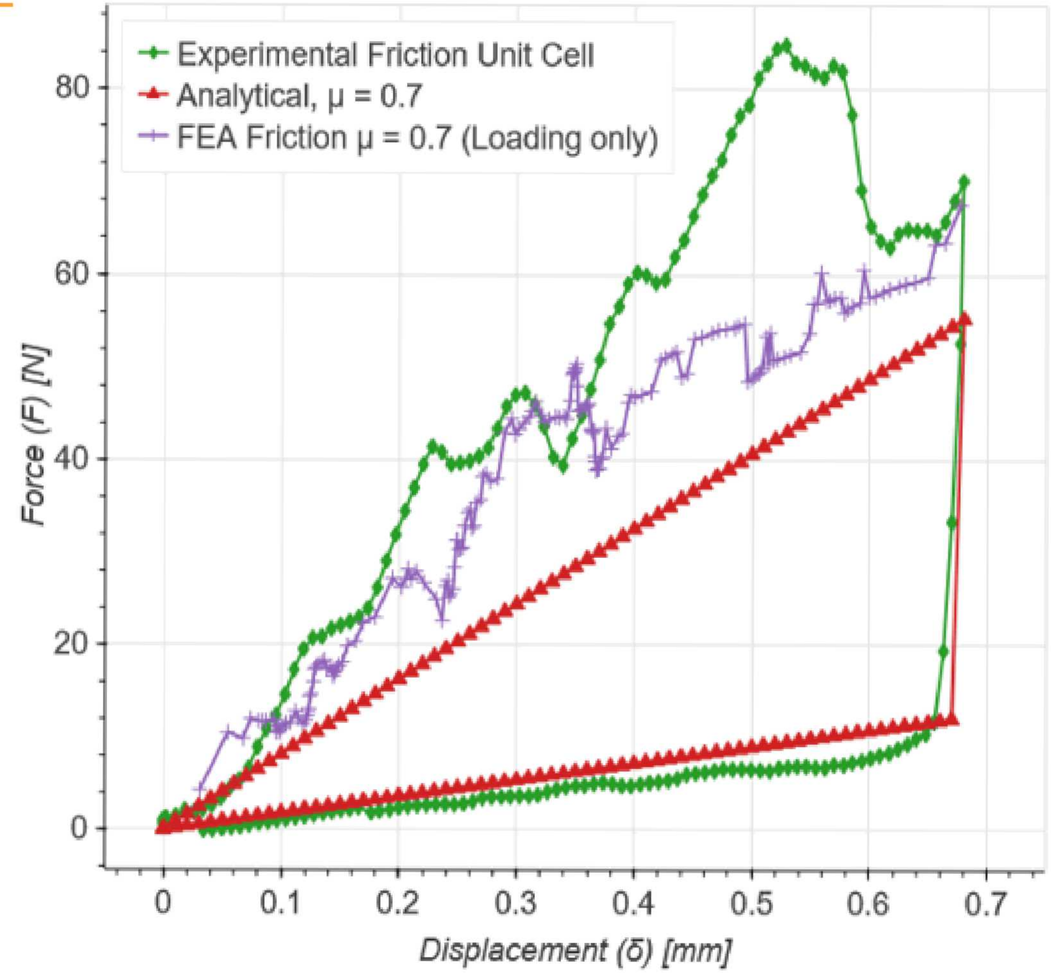
Architecting dissipation at the microscale…





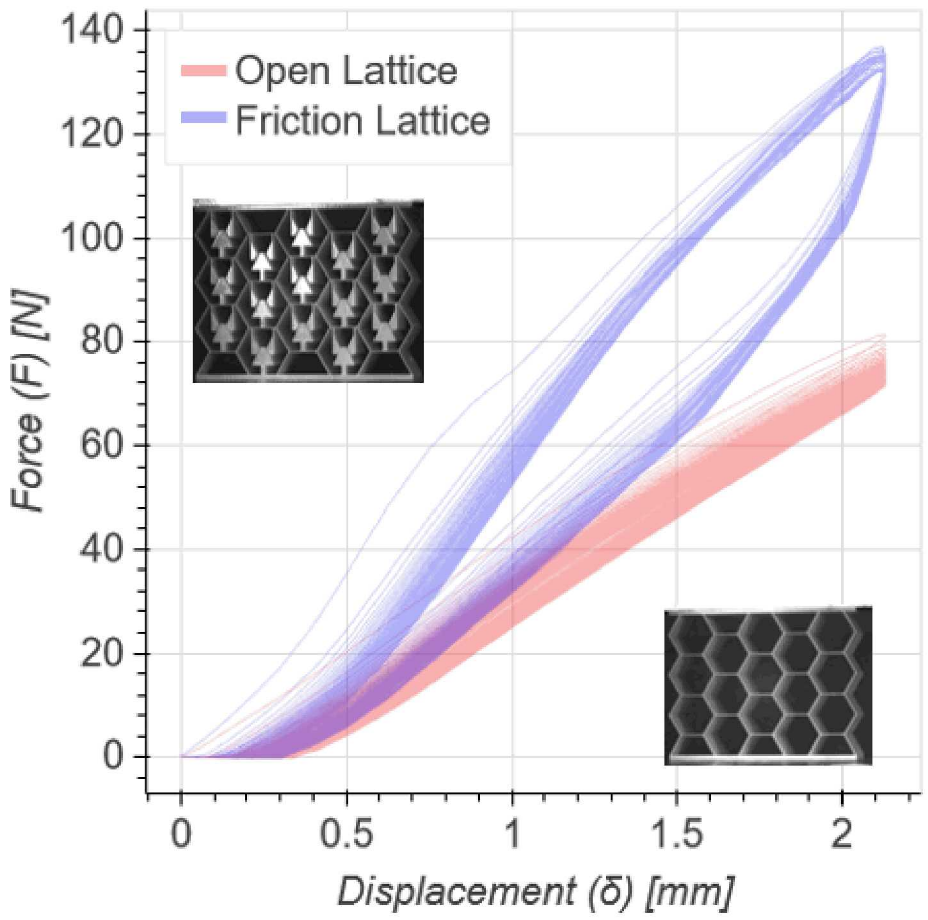
Behavior is predictable = "programmable"

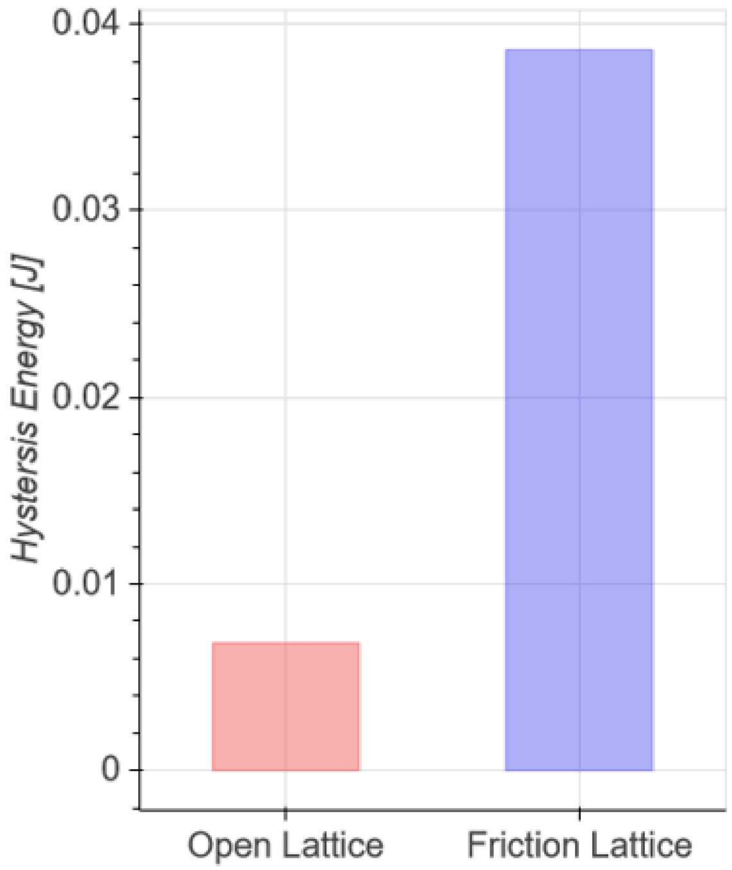




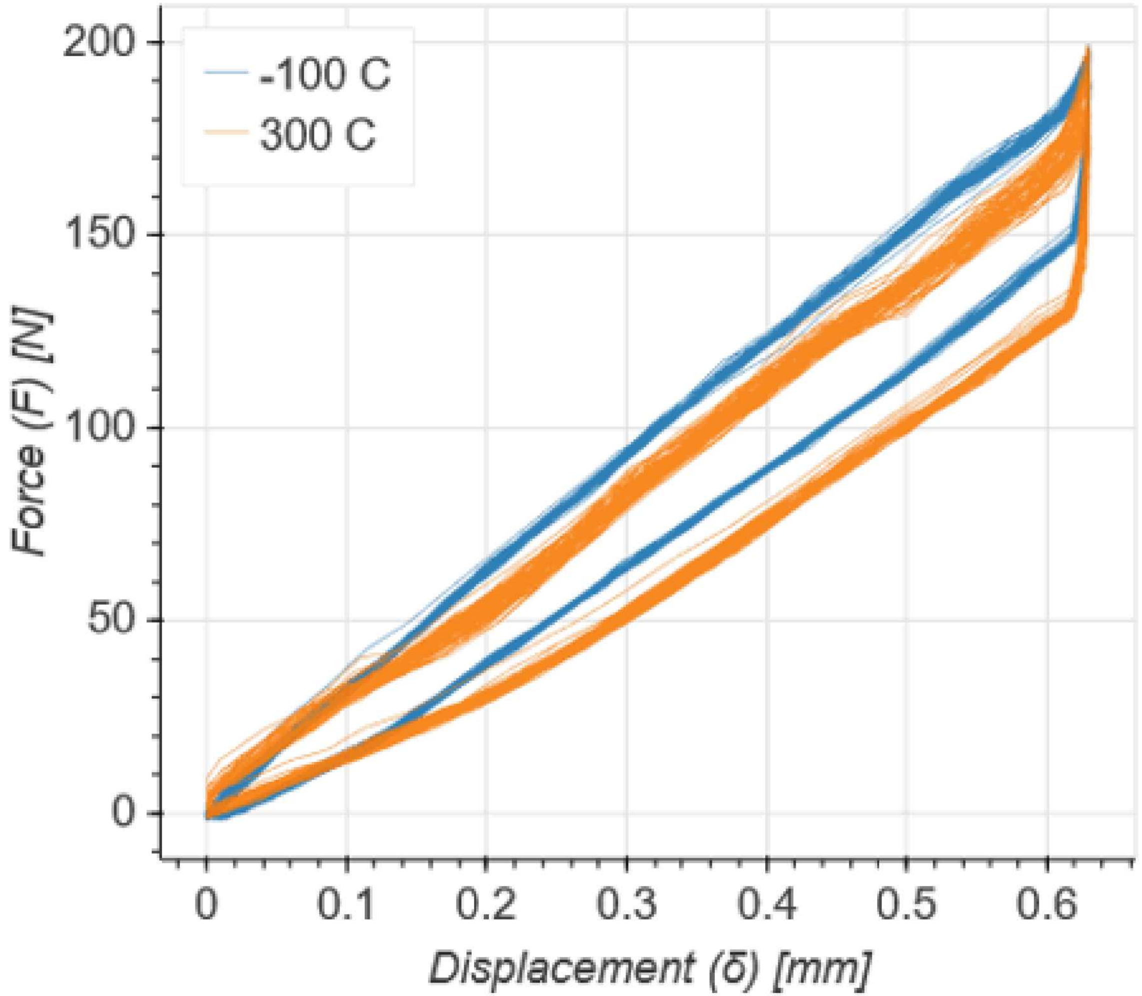
$$W_{FrictionCell} = \frac{EI_{mult} d\delta^2 \mu w^3 \cot(\alpha)\csc(\alpha)\sec(\alpha)}{2(I_{mult}a^3 - a^3 + u^3)} + \frac{EI_{mult} d\delta^2 w^3 \cot^2(\alpha)}{2(I_{mult}a^3 - a^3 + u^3)} + \frac{Ed\delta^2 t^3}{L^3 \sin^2(\theta)}$$

Reusable energy dissipation… like an elastomer

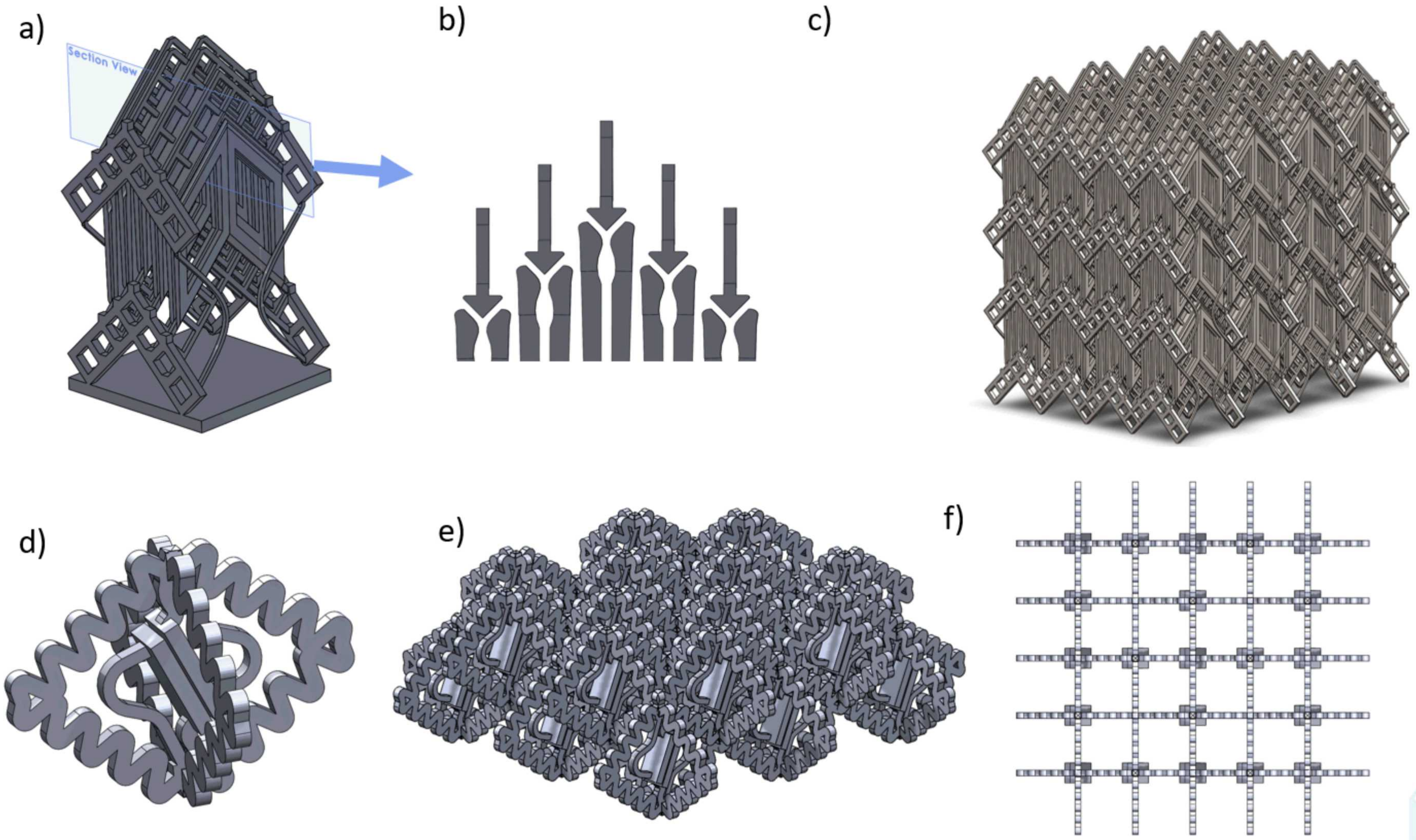




Dissipative properties like an elastomer… but thermally robust…



Complex, hierarchical friction lattices….



Summary…

You can toughen materials with air, but its all about **the placement**!

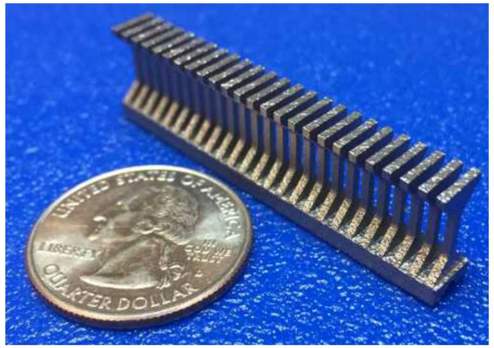
All traditional toughening mechanisms: deflection, delamination, transformation, pull-out, etc. are possible, even with a single material!

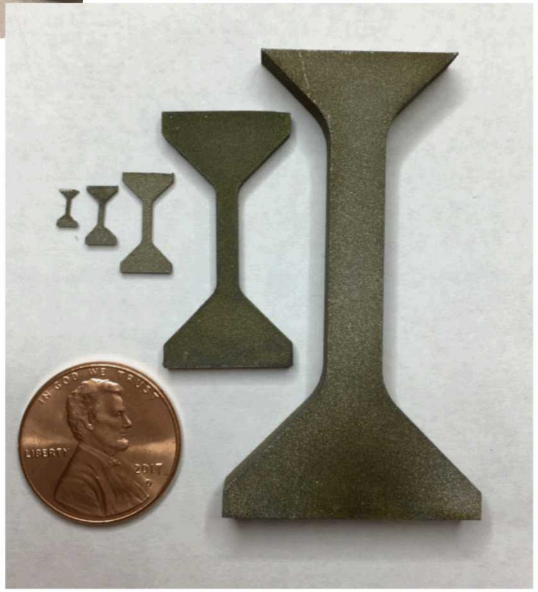
These mechanisms can be enabled *topologically* in any material, albeit with reduced density.

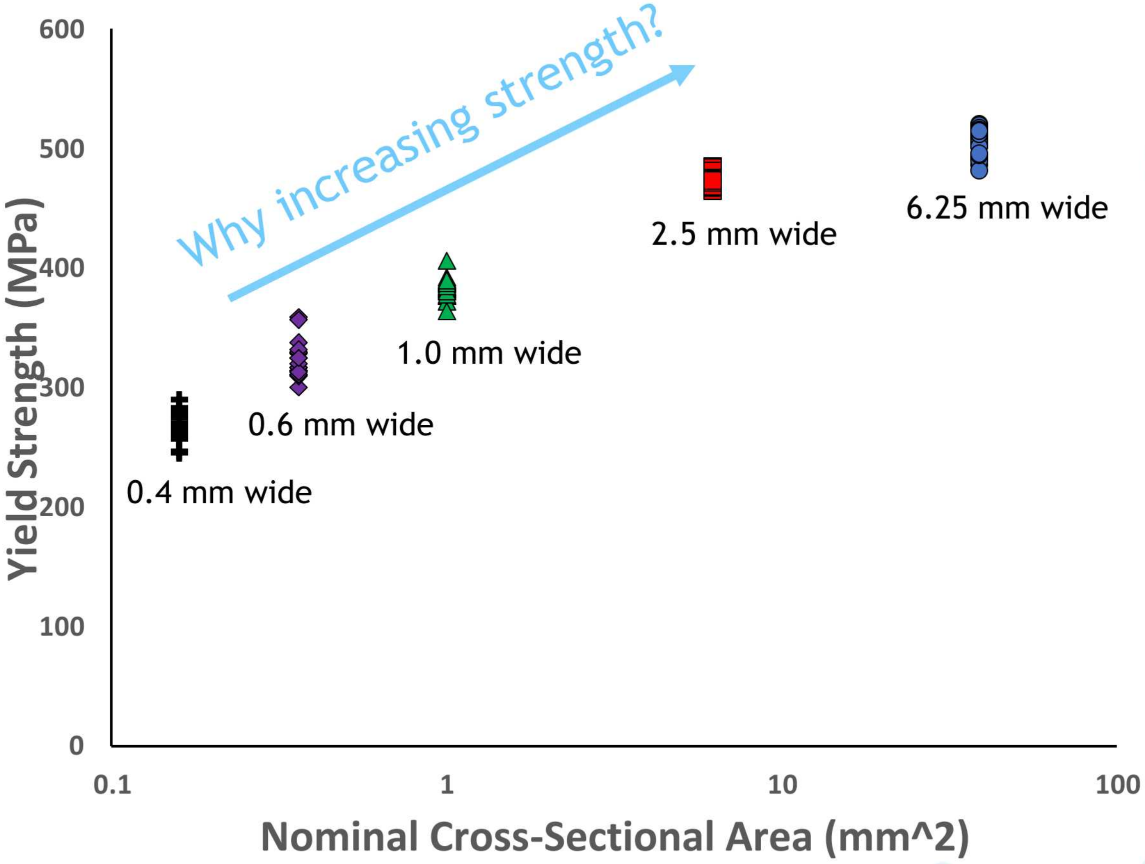
But optimized digital design of fracture resistance is challenging

Setting aside topology… how does it scale?

Representative volume consideration???
Size dependence of effective mechanical properties…

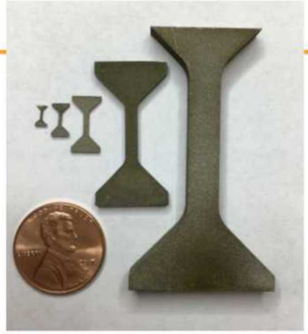


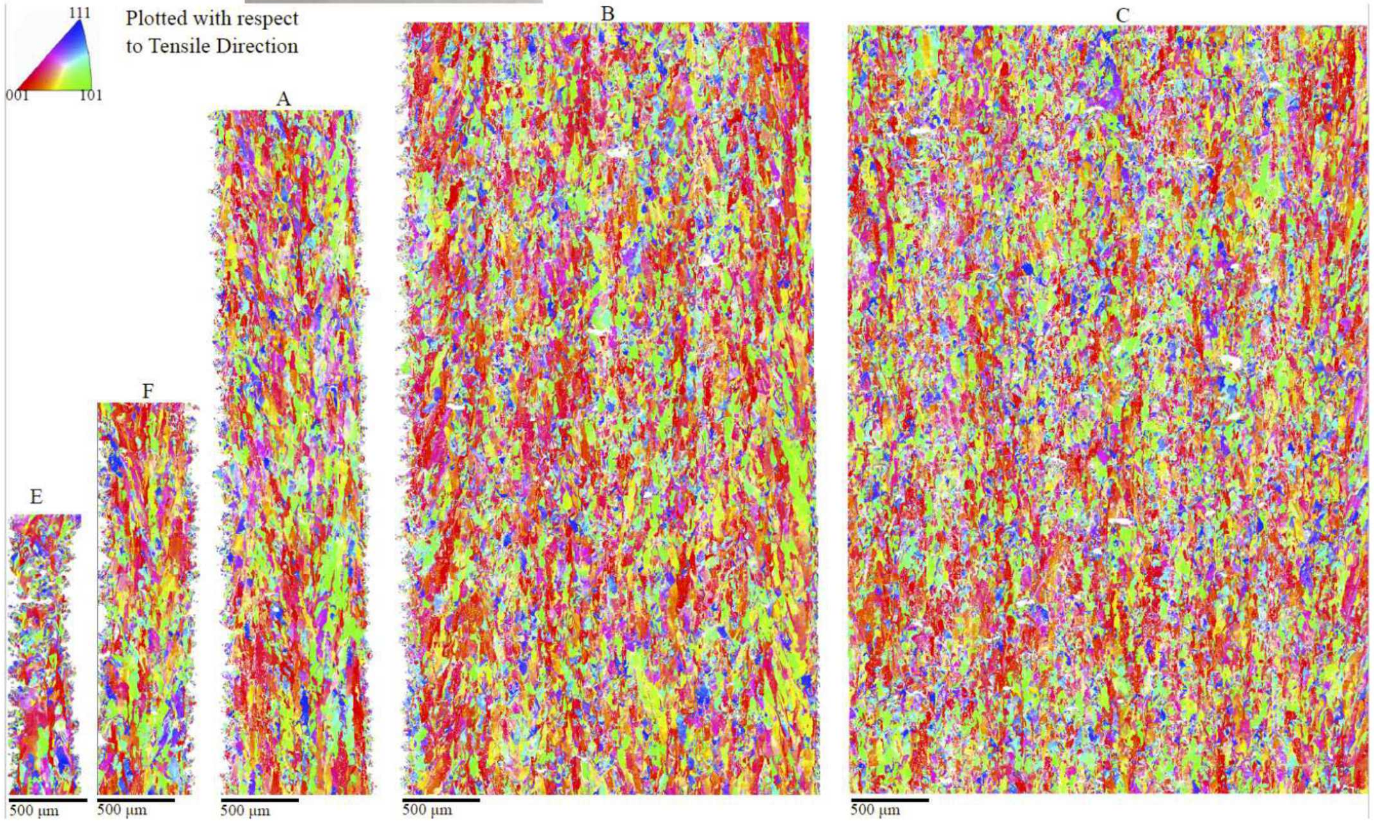


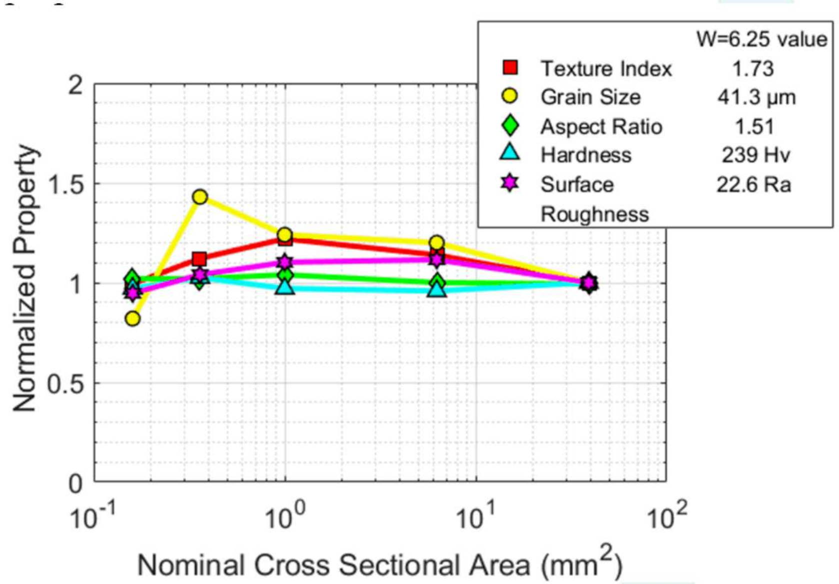


Roach…Boyce, *in review*

No microstructural source of size dependent properties…!

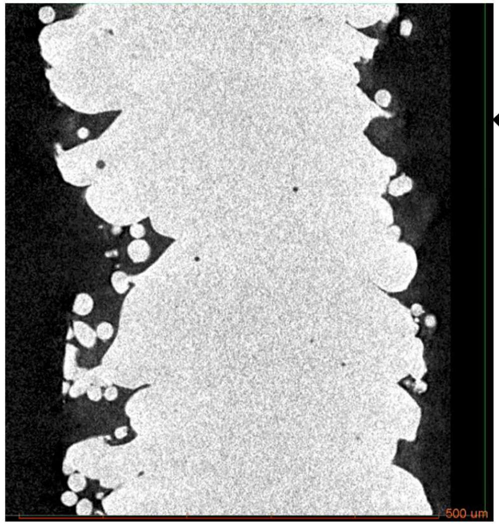


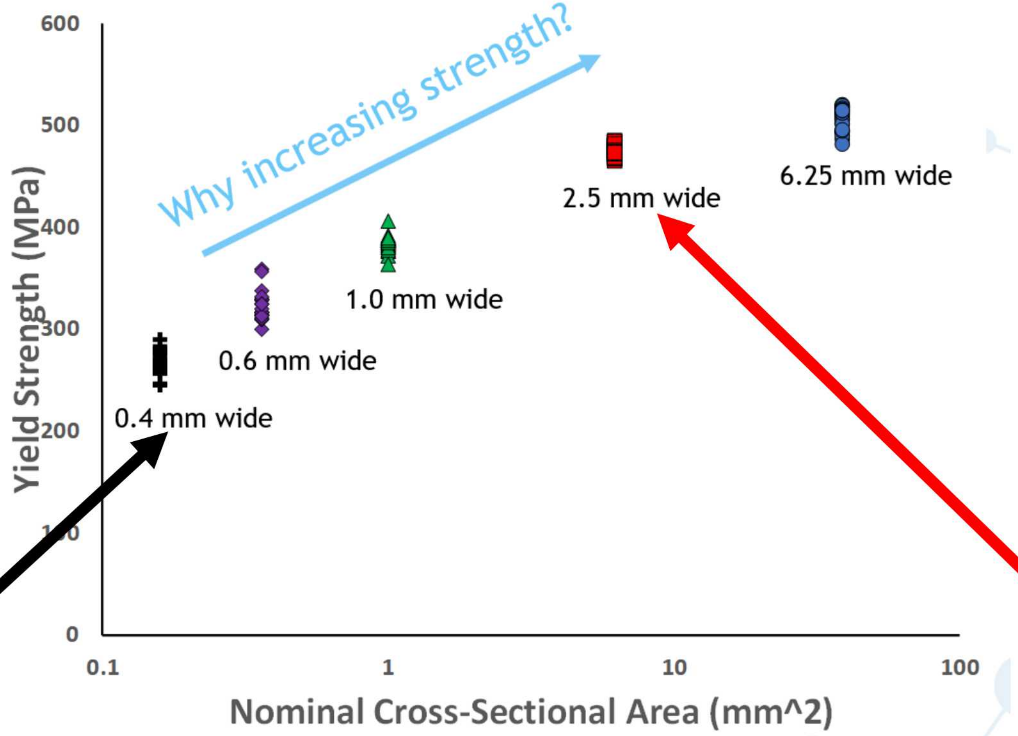


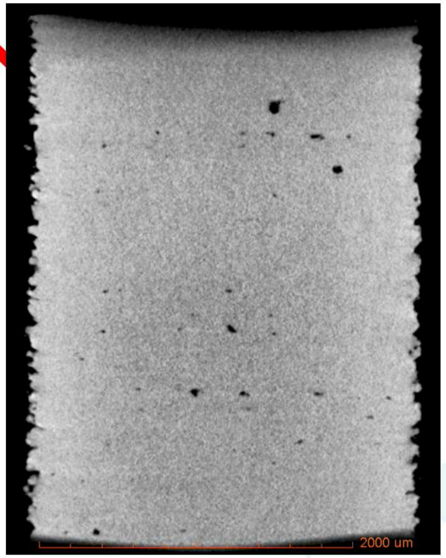


Roach…Boyce, *in review*

Surface topography dominates when features are <2.5 mm!



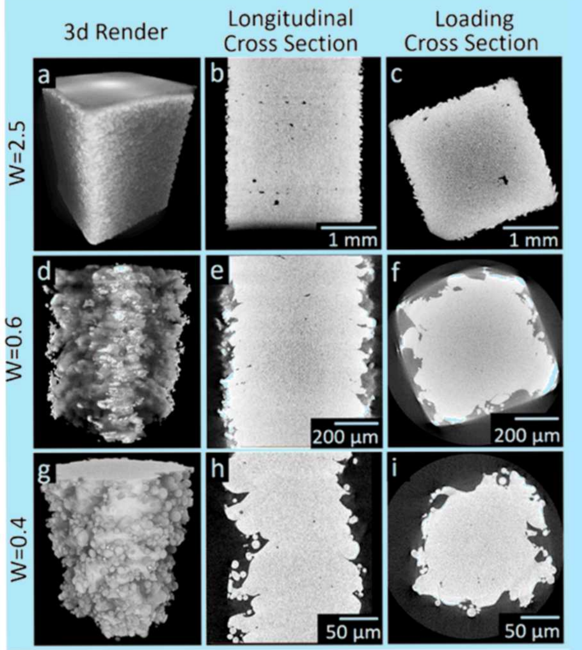




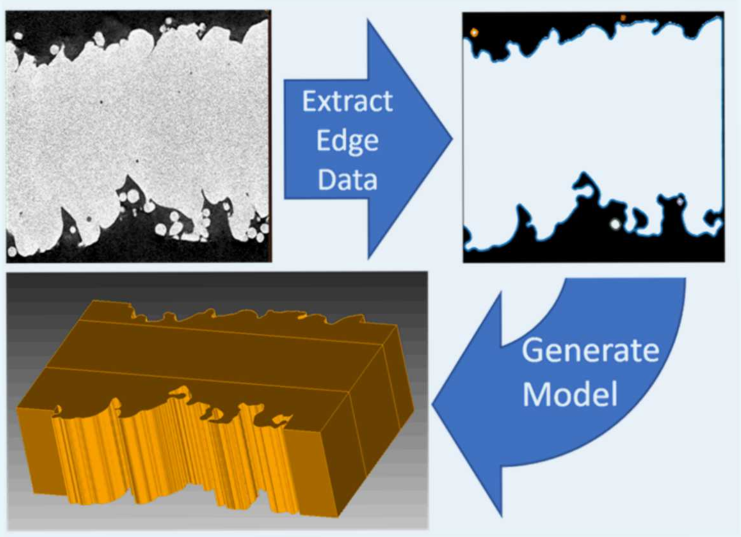
Roach…Boyce, *in review*

Finite element modeling of roughness effect

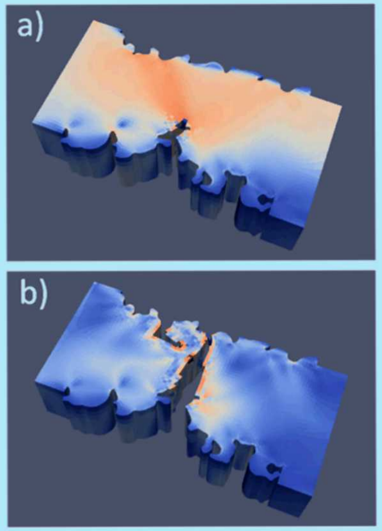
1) Collect CT scans



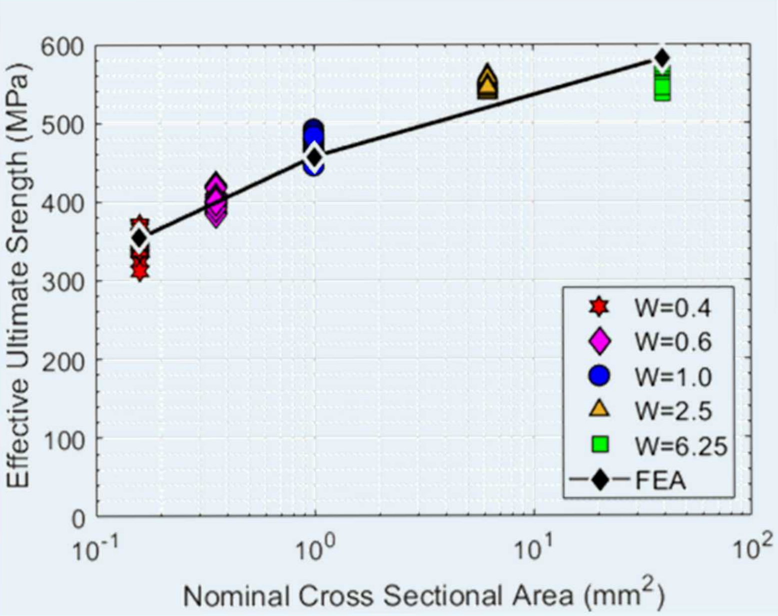
2) Digitize geometry



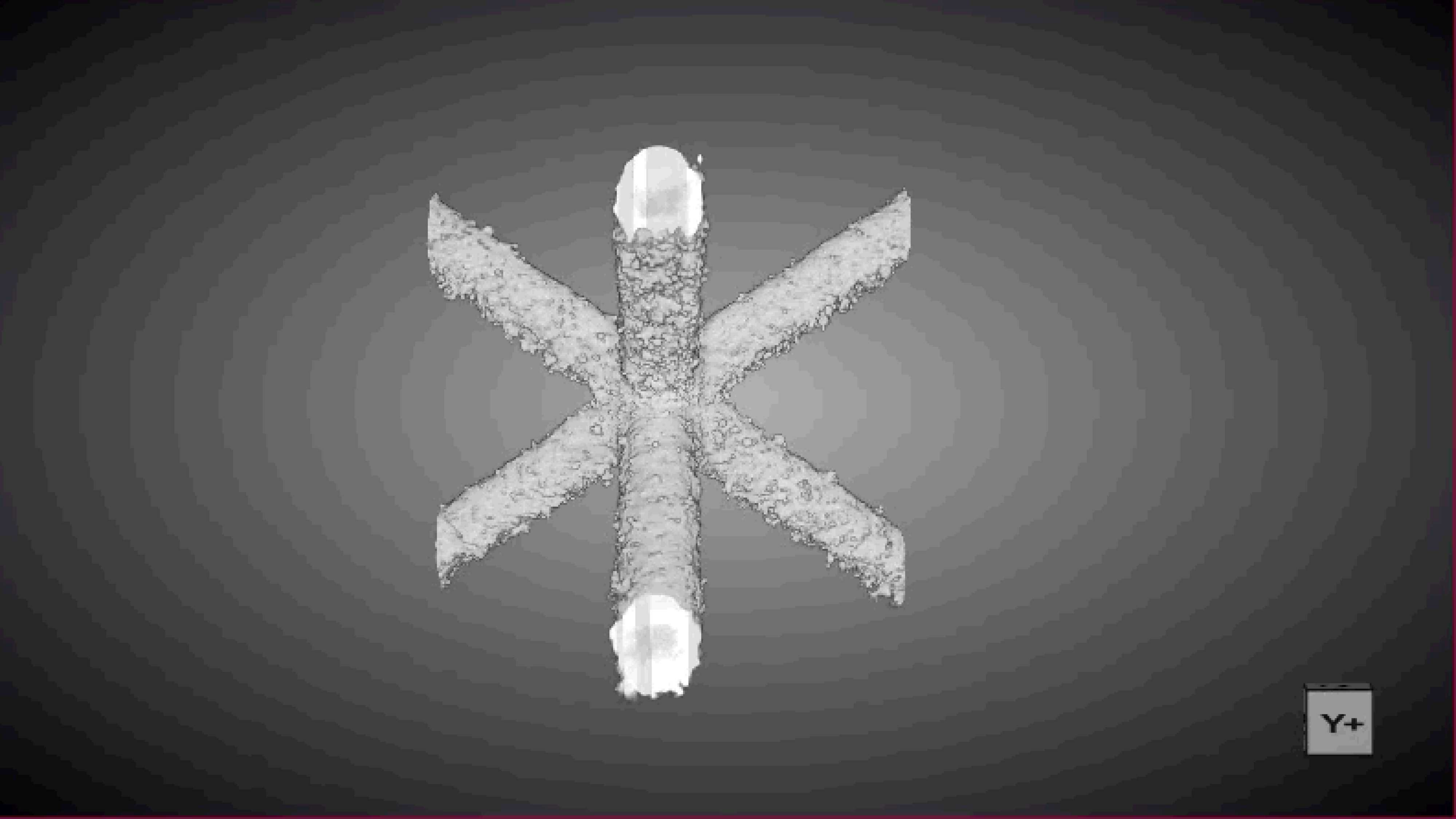
3) FEA



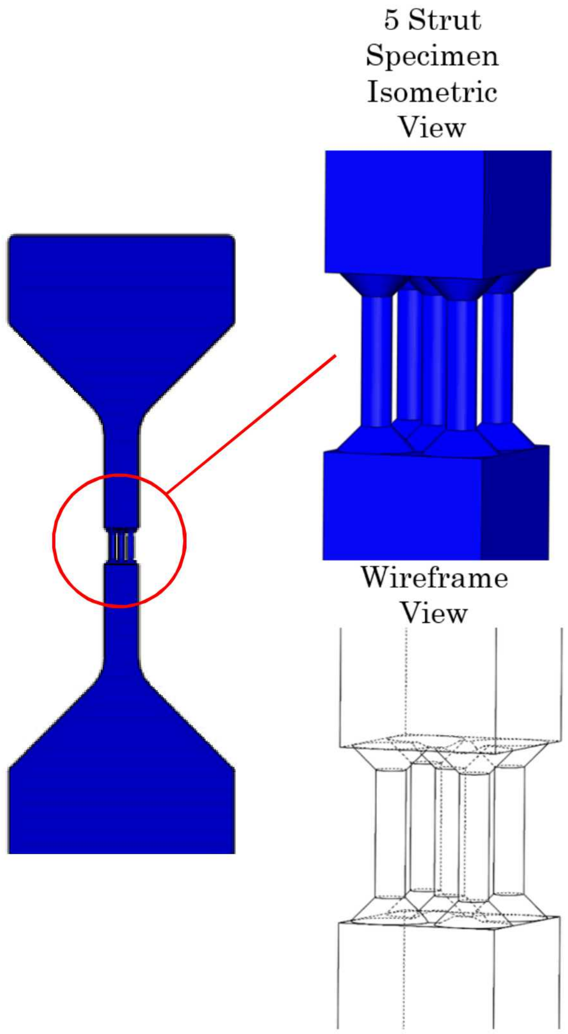
4) Confirm experimental trends

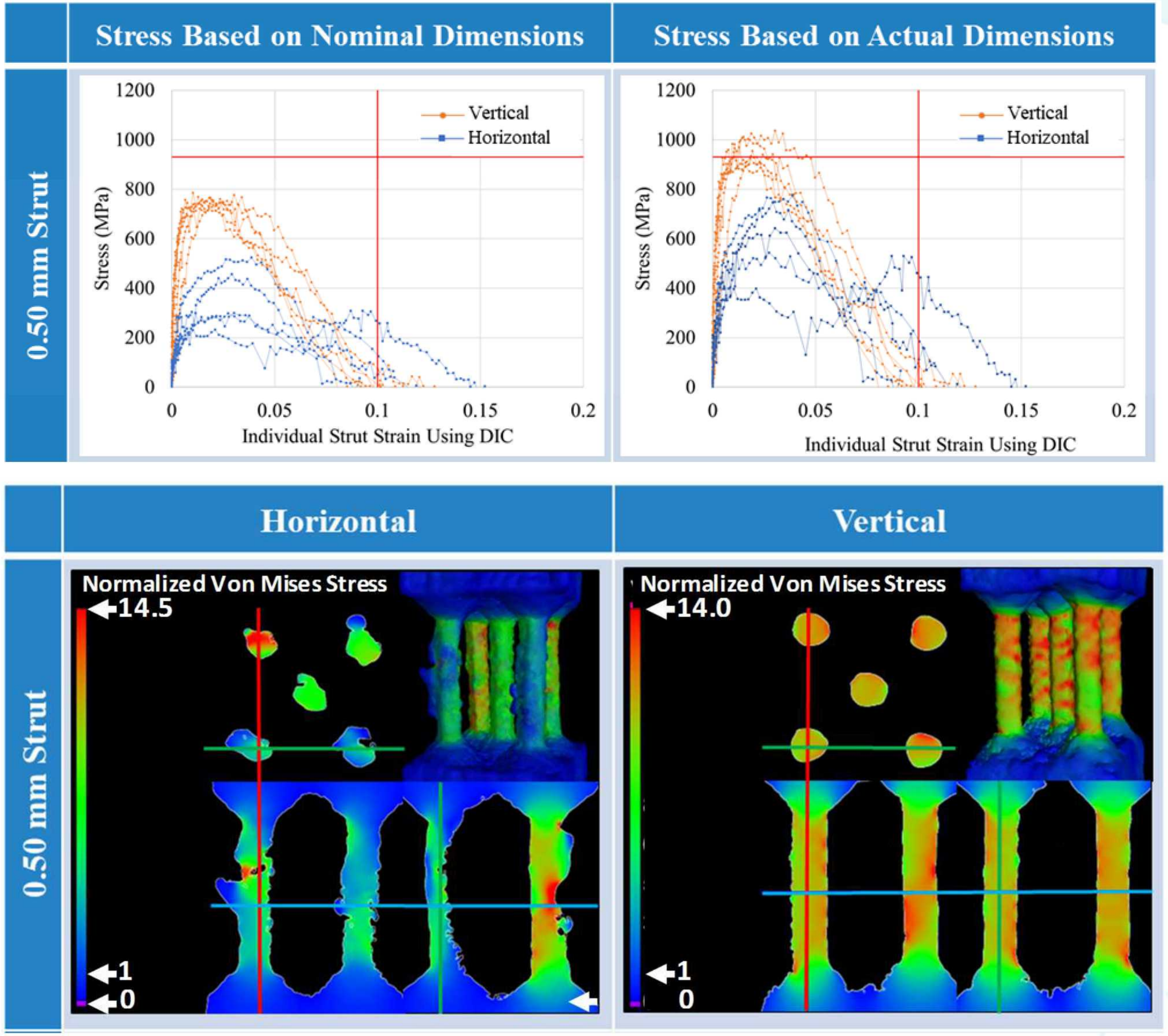


Roach…Boyce, *in review*


Y+

Indeed, the effective strength of struts can be <50% of the 'material' strength

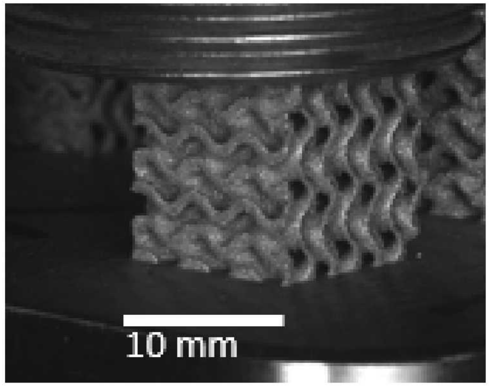


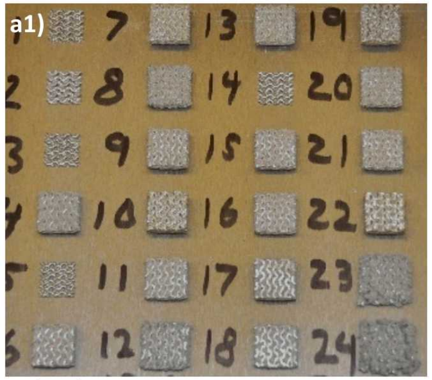


Dressler…Boyce, *Additive Manufacturing*, 2019

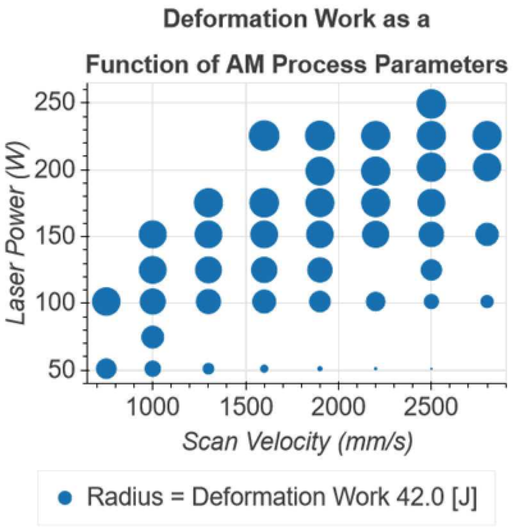
Process parameter study for a lattice…

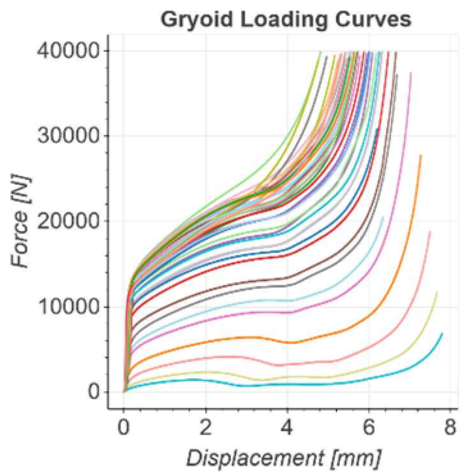
gyroid



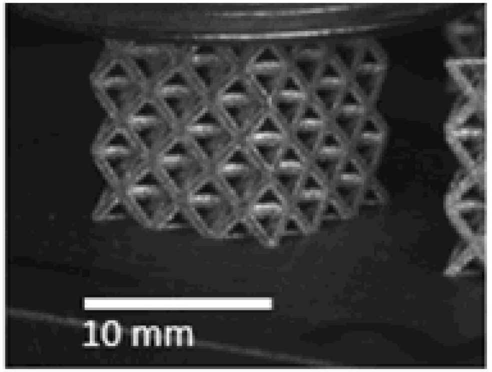


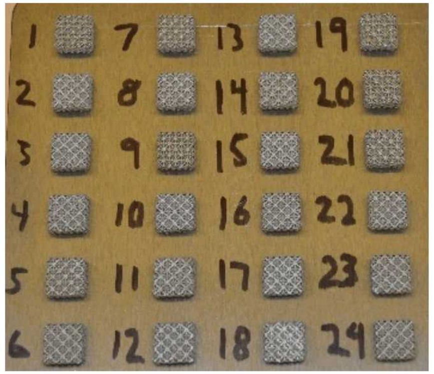
10 mm



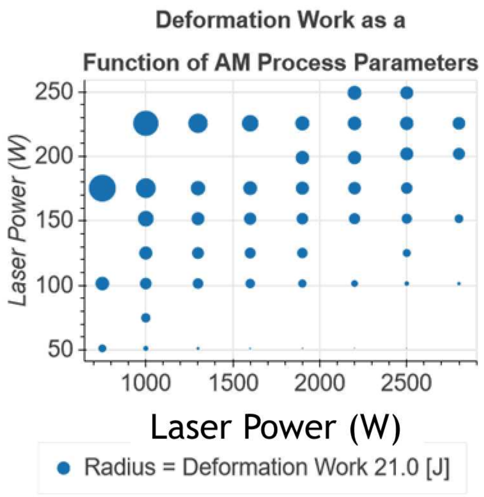


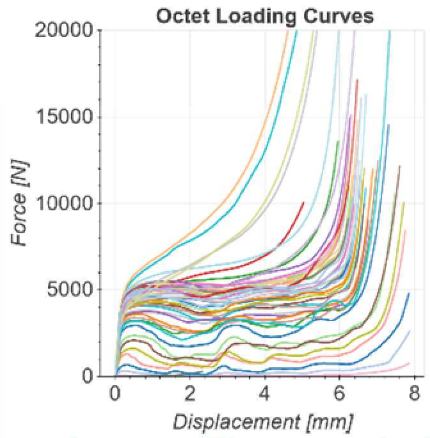
Octet truss





10 mm

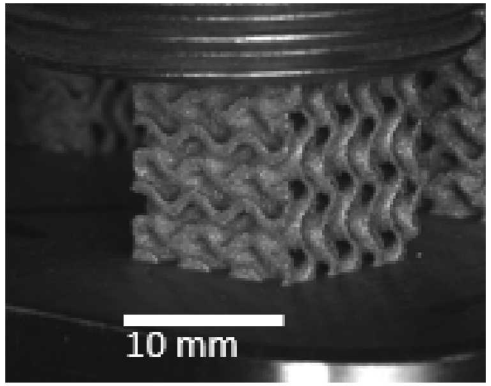


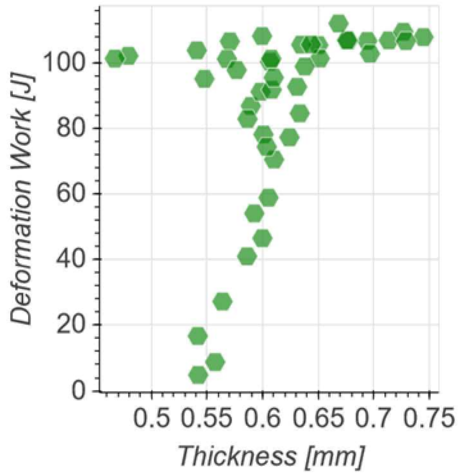


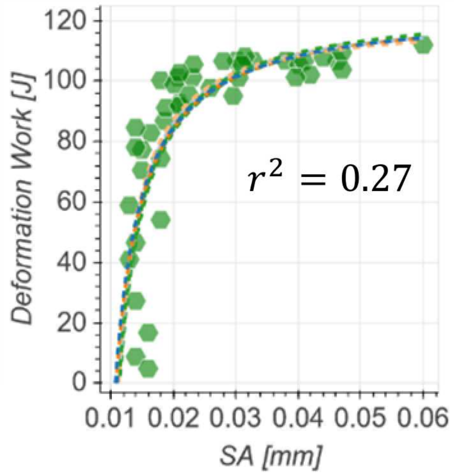
Garland…Boyce, *submitted*

Can we 'predict' mechanical properties with just scalar measures

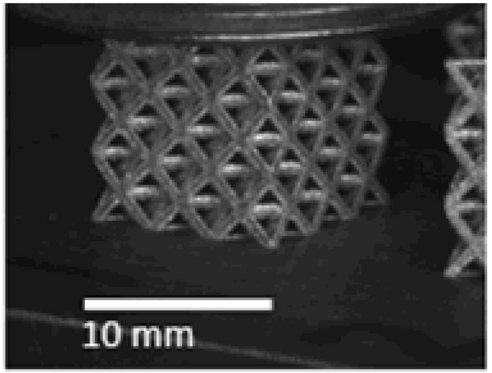
gyroid

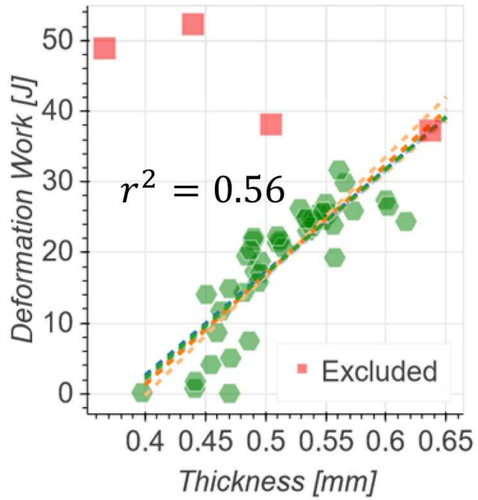


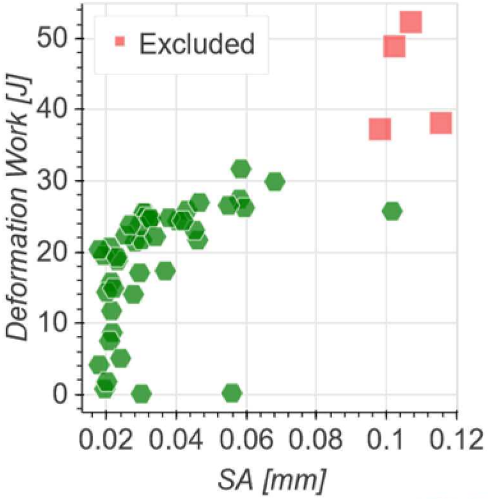




Octet truss



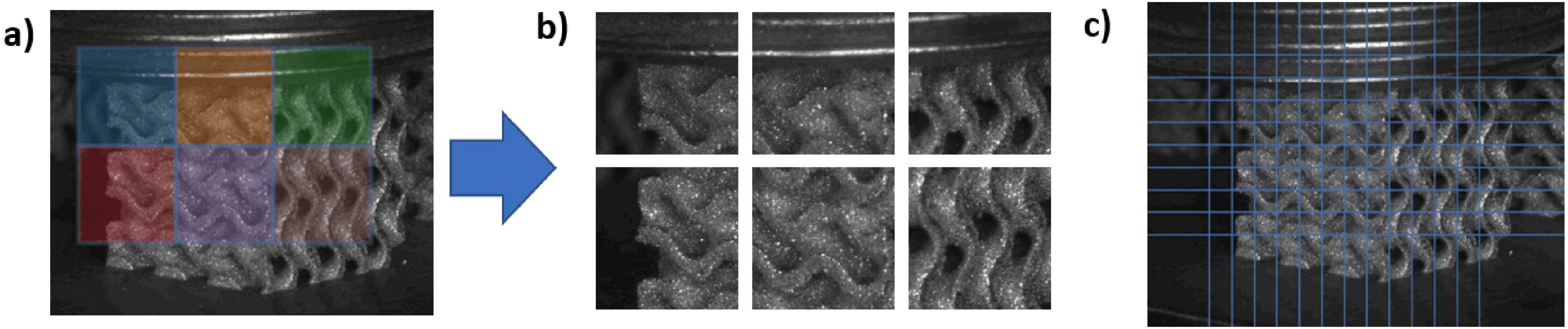




Garland…Boyce, *submitted*

Can machine learning do any better?

Convolutional neural network; 16 layers (resnet16 in fastai library);
stratified k-fold training (8 folds / 11% of data held for testing); enriched data by subwindowing



To ‘enrich’ the available data, rather than training on the entire image, we trained on 45 sub-images (windows) of each original image. This takes advantage of the repetitive nature of the lattice.

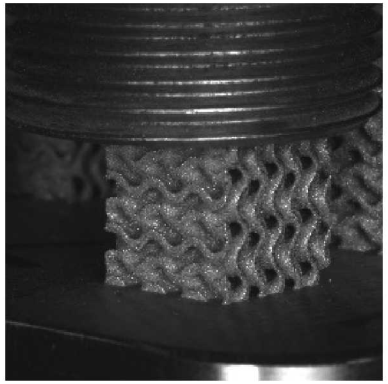
Garland…Boyce, *submitted*

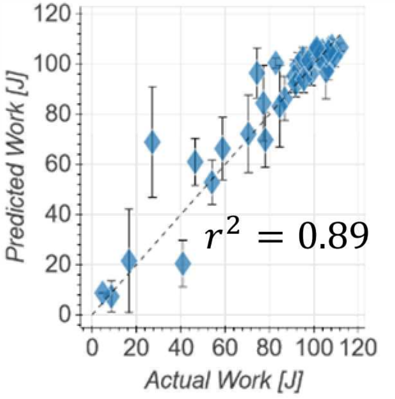
Can machine learning do any better?

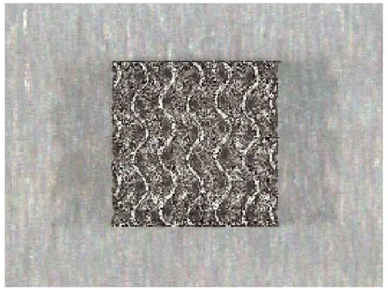
Oblique view

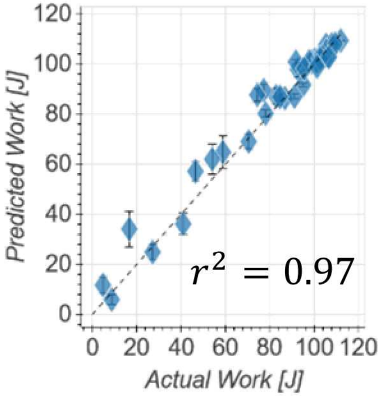
Top-down view

gyroid

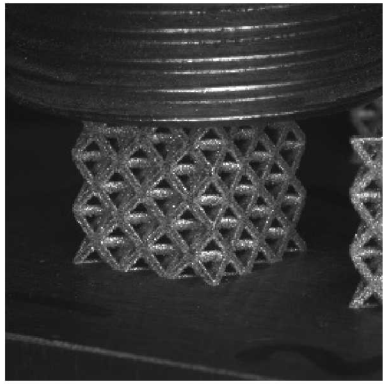


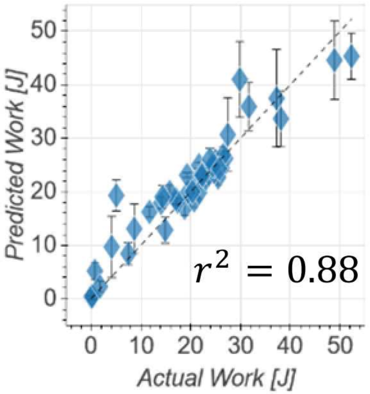


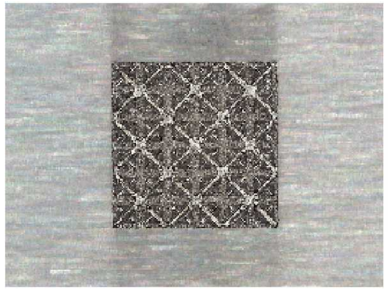


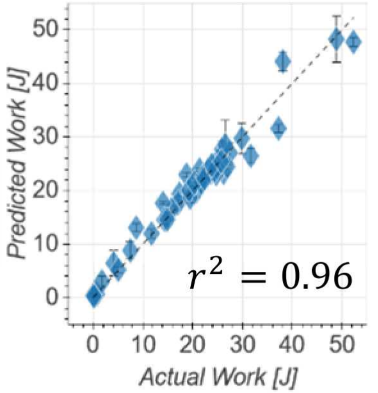


Octet truss



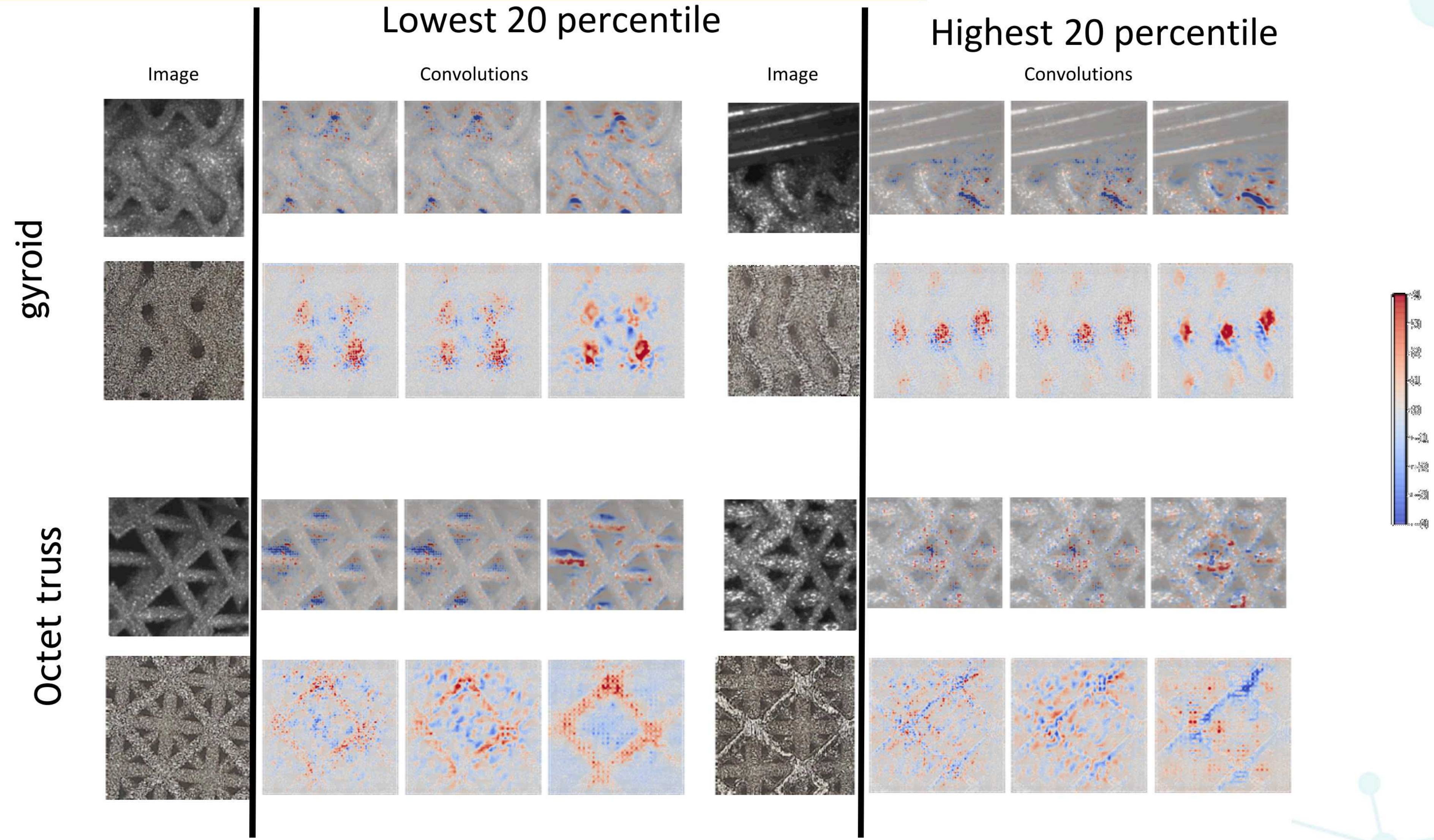






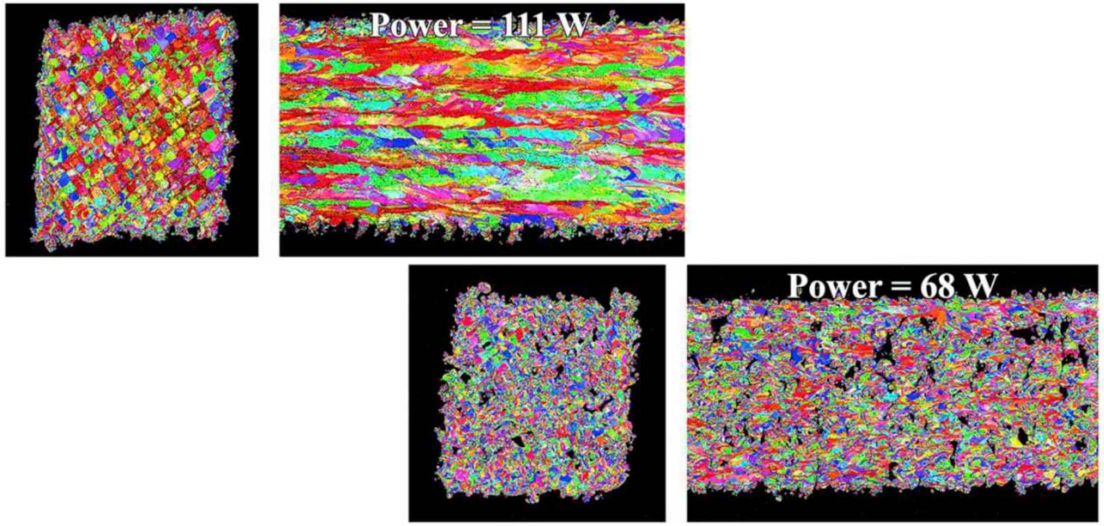
Garland…Boyce, *submitted*

Machine learning's weakness: '*explainability*' and *extrapolation*

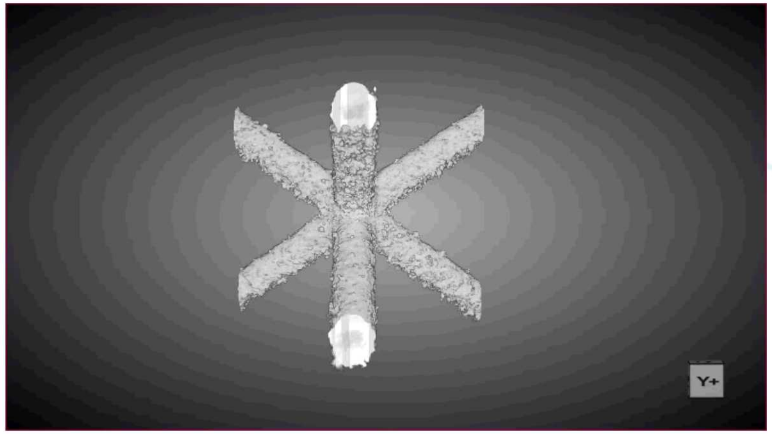


Summary

Monolithic AM



Feature-rich AM



First order influence: microstructure & porosity

Complex pathway to prediction

First order influence: dimensions & surface topography

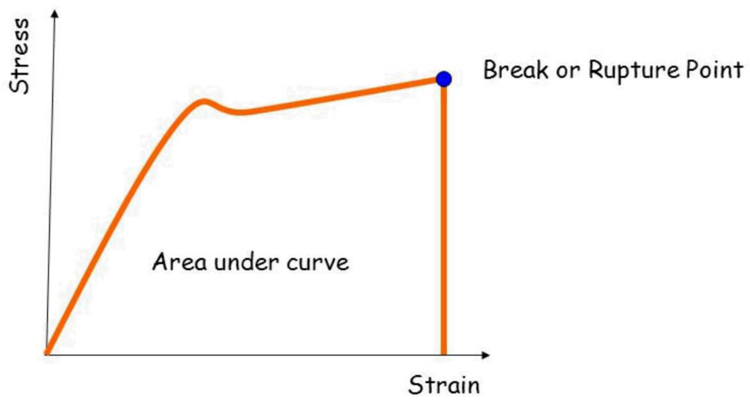
Potentially easier to predict

In this presentation, I drew data from ~2000 mechanical tests. High-throughput testing and machine learning enable us to develop process-structure-property relationships that were otherwise elusive.

Toughness: two basic definitions

Toughness = work of fracture

Units of J or N-m

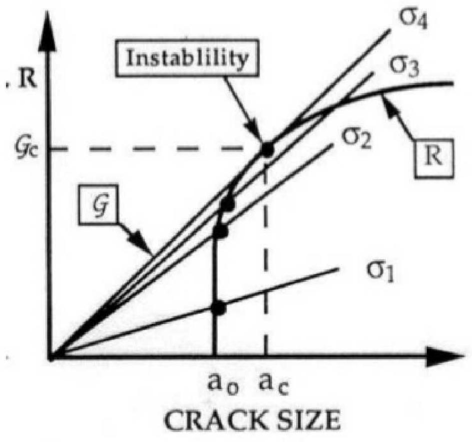


$$W = \int \mathbf{F} \cdot \mathbf{dx}$$

$$U = \int \boldsymbol{\sigma} : d\epsilon \, V$$

Fracture toughness= work required advance a crack by a unit length

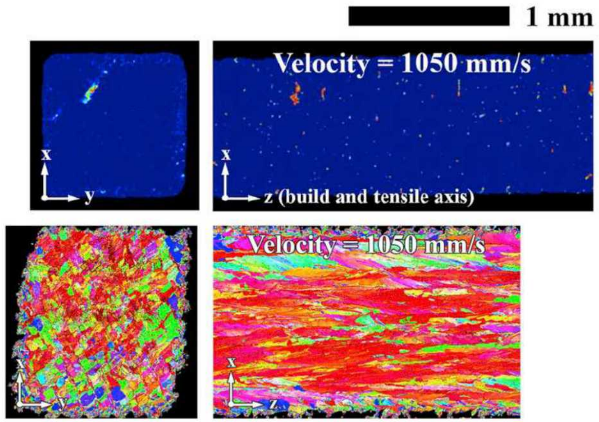
Units of MPa√m (K) or J/m^2 (G)



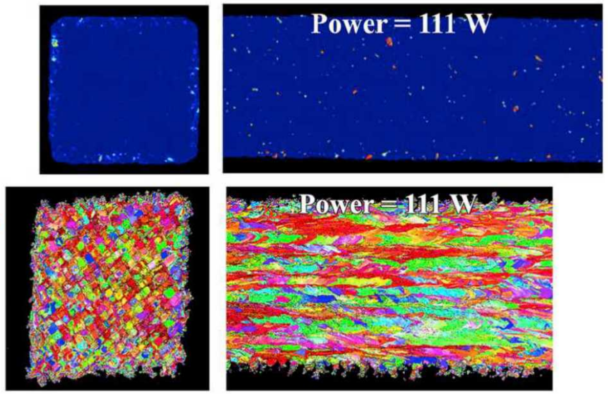
$$G = G_I = \begin{cases} \dfrac{K_I^2}{E} & \text{plane stress} \\ \dfrac{(1-\nu^2)K_I^2}{E} & \text{plane strain} \end{cases}$$

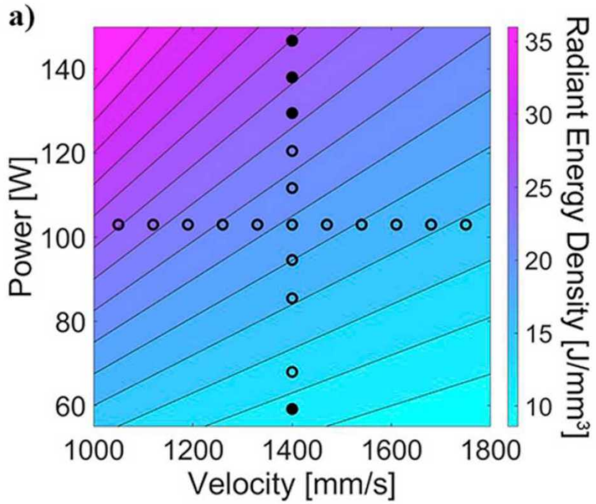
Process parameter study

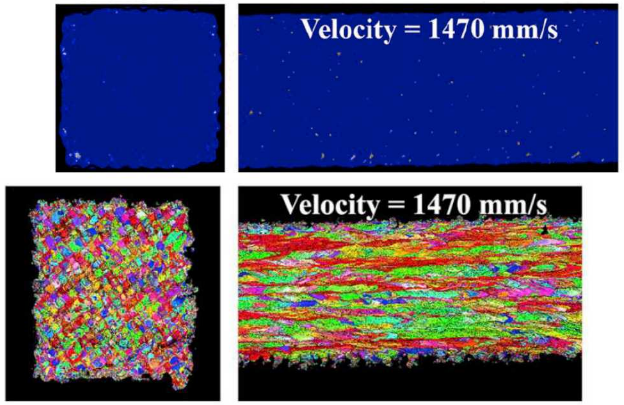
X-ray computed tomography

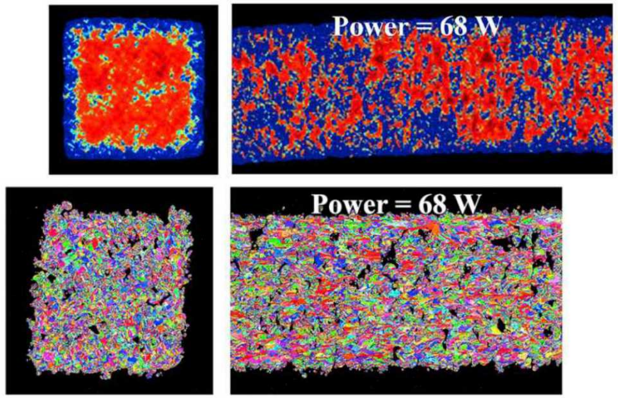


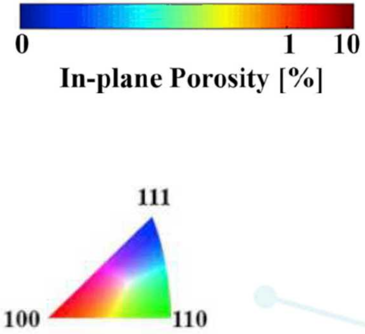
High-speed electron backscatter diffraction





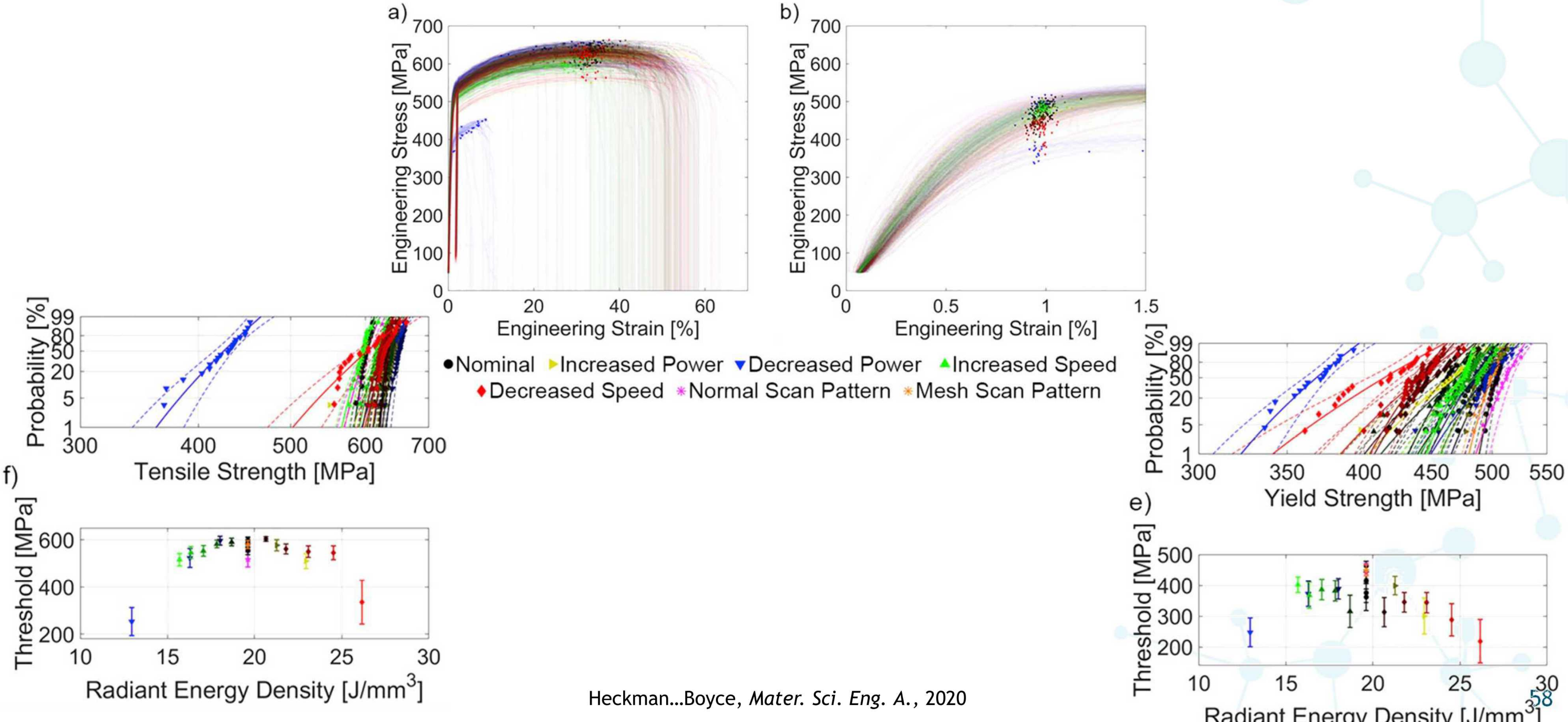






Heckman…Boyce, *Mater. Sci. Eng. A.*, 2020

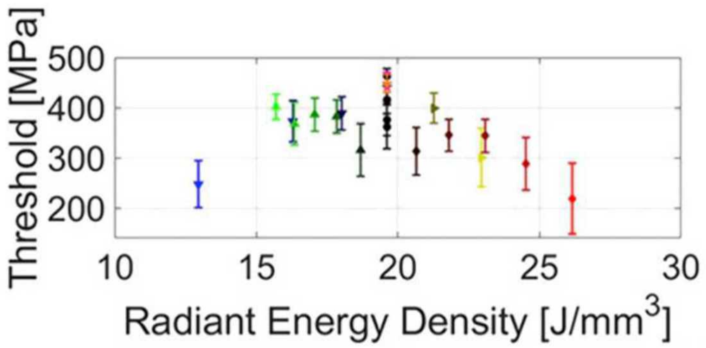
High-throughput data → a Weibull minimum allowable threshold

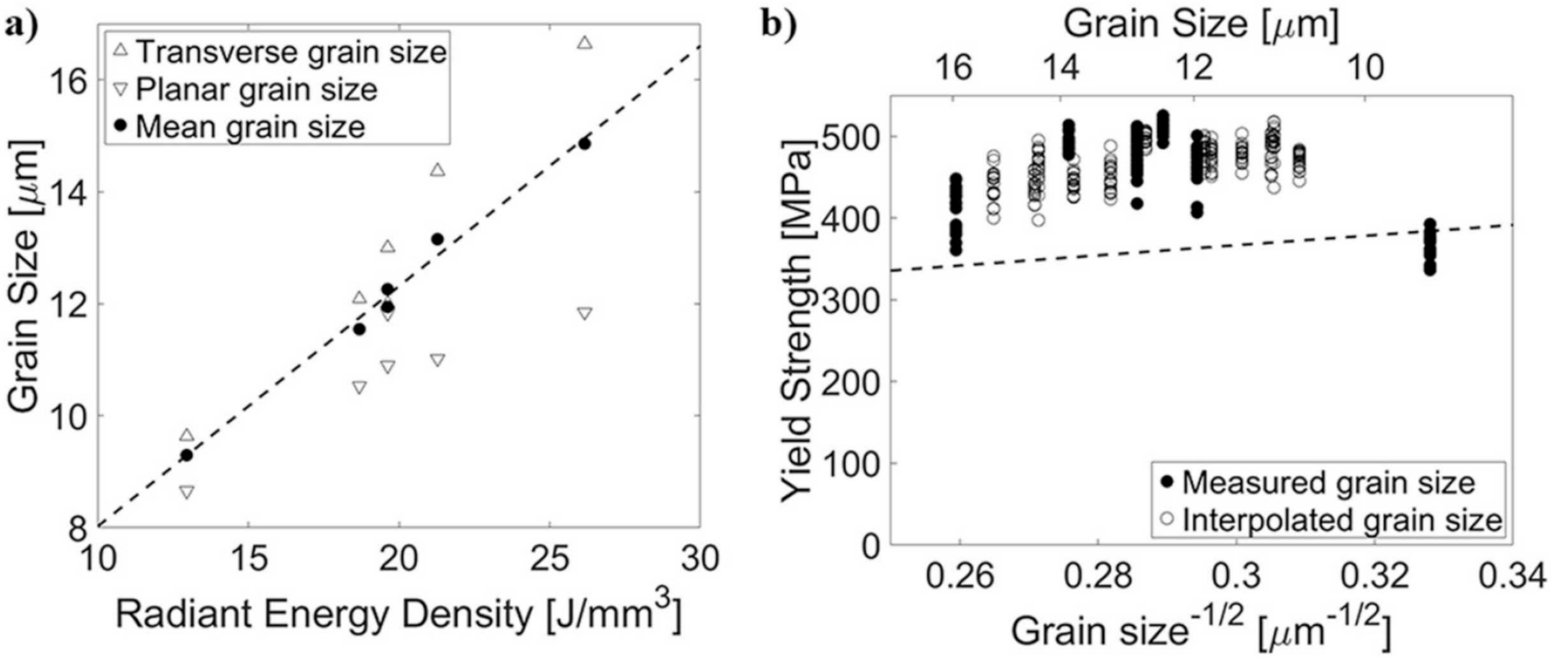


Heckman…Boyce, *Mater. Sci. Eng. A.*, 2020

Connecting the dots… the old fashioned way…

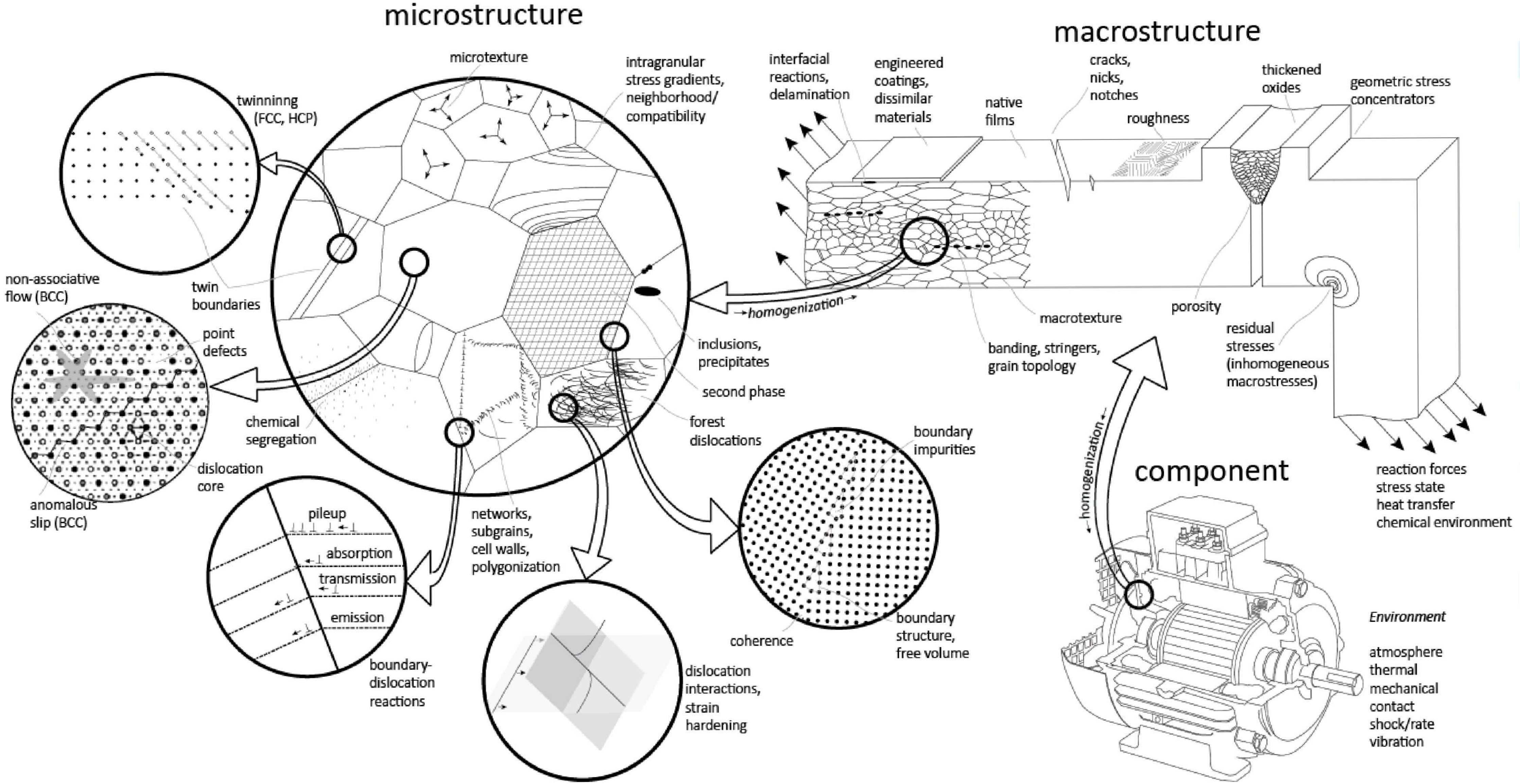
Weibull threshold
Yield Strength (MPa)





Heckman…Boyce, *Mater. Sci. Eng. A.*, 2020

Grain size is not the only factor affecting mechanical response…



Griffith fracture criterion (1921)[2]

Criterion: Crack growth will occur if the potential energy decrease produced by an increment of crack extension equals the energy needed to extend the crack that same increment.

$$\sigma = \sigma_f, \text{ if } \frac{\partial \Pi}{\partial a} = \frac{\partial W}{\partial a}$$

For the elliptical crack

$$\frac{\partial \Pi}{\partial a} = \frac{\pi a^2 \sigma_0^2}{E^*}, \quad E^* = \begin{cases} E, & \text{if plane stress} \\ \frac{E}{1-\nu^2}, & \text{if plane strain} \end{cases}$$