Mechanics of soft composites: From deployable structures to self-organized patterns

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Structures traditionally seen as a system of connected parts with the goal of bearing a load while maintaining shape.

Structural mechanics applied now much more widely.
Materials with engineered microstructure

The line between material and structure is no longer clear.
Structures now make use of the nonlinear regime

Flexible  Active  Multiphysics

Harnessing instabilities  Biological systems
Materials with engineered microstructure + Nonlinear mechanics of soft solids

Cellular solids

Flexible fiber composites

Patterns on soft solids

Granular media

Textiles

Materials optical attenuation
FLEXIBLE FIBER COMPOSITES

Collaboration with:

Prof. Sergio Pellegrino (Caltech)

Dr. Juan Mejia-Ariza (L’Garde)

Prof. Oscar Lopez-Pamies (UIUC)
Deployable methods, especially for precision large rigid structures or flexible materials are the enabling force behind developing the larger systems needed to attain advancements in science and engineering of today and tomorrow.

NASA Space Technology Roadmap, 2012
Traditional deployable structures are rigid and require mechanical elements:

- Complex
- Heavy
- Expensive
- External actuation

MOTIVATION

NuSTAR – Space x-ray telescope (caltech.edu)

Folded mast (atk.com)

Stowed mast in canister (atk.com)
An alternative are structures that deform elastically during packing.

The structure self deploys releasing strain energy.

Designs are limited by the curvature failure of the material.
Fiber composites with a very soft elastomeric matrix can be folded to very high curvatures without breaking.

Fiber composite Miura-Ori pattern (Maqueda et al., 2012)

Why does this happen?

Does it have any effect on the material?

How tightly can we pack the composite?
WHY DOES THIS HAPPEN?

When folded, the fibers microbuckle without breaking. Fiber microbuckling acts as a stress relief mechanism.
**EXPERIMENTAL CHARACTERIZATION**

**HTS40-12K carbon fibers (TohoTenax)**
Diameter: 7 μm  
Tensile modulus: 240 GPa  
Failure strain: 1.8 %

**CF19-2615 silicone (NuSil Technology)**
Initial tensile modulus: 1 MPa  
Failure elongation: 120% – 140%  
No viscoelastic behavior or Mullins effect observed.
Bending behavior:

- Highly nonlinear
- Strain softening and hysteresis under cyclic loading

\[ \kappa = 0.21 \text{ mm}^{-1}, \quad \kappa = 0.29 \text{ mm}^{-1}, \quad \kappa = 0.35 \text{ mm}^{-1} \]
EXPERIMENTAL CHARACTERIZATION

It is hard to decouple material effects from the nonlinearities due to microbuckling.

Tension perpendicular to the fibers isolates the effects of damage.

Behavior close to typical filled rubber (Mullins effect).
Finite element model in Abaqus/Standard:

• Representative volume element (RVE) with periodic boundary conditions

• Continuum elements used for both fiber and matrix

• Gent hyperelastic model for the matrix, fitted from tensile experiments:

\[ W = -C_1 J_m \ln \left( 1 - \frac{J_1}{J_m} \right) + C_2 \ln \left( \frac{J_2 + 3}{3} \right) \]

• Different fiber distributions used:
  - Purely random
  - Random based on micrographs
FINITE ELEMENT MODELING

Usual idealizations

Square

Hexagonal

Random
(Poisson process)

Reality

$V_f = 65\%$

$V_f = 22\%$
The fibers can be used to calculate the second order intensity function $K(r)$ (Pyrz, 1994)

It measures the average number of fibers within a radial distance from an arbitrary fiber:

$$K(r) = \frac{A}{N^2} \sum_{k=1}^{N} w_k^{-1} I_k(r)$$

- $A$: Area considered
- $I_k(r)$: Number of fibers inside a circle of radius $r$
- $N$: Total number of fibers
- $w_k$: Factor introduced to correct edge effects

Reconstruction algorithm (Rintoul and Torquato, 1997) minimizing the following energy:

$$E = \sum_{k} \left( K(r_k) - \bar{K}(r_k) \right)^2 + \sum_{i} \sum_{j} \left( \left( \frac{100}{d_{ij}} + 10 \right) \delta_{ij} + 100 \delta_i \right)$$
Microstructure affects the stress and strain concentrations.

This is very important to model the damage process.

Examples with $V_f = 50\%$
The simulation can only capture the initial stiffness.

Cohesive elements introduced to model the damage due to debonding.
Model with cohesive elements captures:

Nonlinearity.

Damage under cyclic loading (no hysteresis)

Dependence on fiber volume fraction

$V_f = 65\%$

$V_f = 22\%$

FLJ and Pellegrino, IJSS, 2012
The model predicts a reduction in fiber strain.

However, this effect is not enough to explain the performance of the material.

\[ V_f = 30\% \]
\[ \kappa = 0.35 \text{ mm}^{-1} \]
The same happens when single carbon fibers under bending.

This is done with the fiber loop test (Sinclair, 1950):

Assuming $\varepsilon = \kappa \cdot r$, the maximum strain at A is much higher than the fiber failure strain under uniaxial tension.
Carbon fiber as a very complicated structure.

Failure is probabilistic in nature, and depends on the presence of flaws.

Bennet and Johnson (1978)
FIBER FAILURE

Under bending the stress is highly localized, so curvature failure is higher than expected.

Can we connect tension and bending?
Brittle failure is modeled with a Weibull distribution:

\[ P(\sigma, V) = 1 - \exp \left( -\frac{V}{V_0} \left( \frac{\sigma}{\sigma_0} \right)^m \right) \]

\( V_0 \) – volume dependence
\( \sigma_0 \) – normalizing stress

The Weibull modulus \( m \) describes the variability in strength:
Testing of single fibers provides a description of the failure process.

\[ \sigma_0 = 4.68 \text{ MPa} \]

\[ m = 10.397 \]

\[ \varepsilon_0 = 1.89 \% \]

However, this equation is a simplification for pure tension.
For general loading:

For pure bending: \( \sigma = E_t \kappa \eta \)

Loop test can be analyzed using Euler’s elastica.

Failure as function of curvature
In the case of fiber microbuckling in the composite:

Wavelength:

\[ \lambda = \lambda_0 (1 - \kappa t) \]

\[ \lambda_0 = \left( \frac{9\pi^3 V_f t^2 EI}{8R^2 \log \left( \frac{3t}{b} \right) G} \right)^{\frac{1}{4}} \]

Francis et al., 2007

Amplitude:

\[ \int_0^1 \sqrt{1 + \left( \frac{a}{\lambda} \pi \cos \pi \hat{x} \right)^2} \, d\hat{x} = \frac{1}{1 - \kappa t} \]

To compare, specimens of 0.5 mm thickness folded to different curvatures. We then calculate the percentage of broken fibers.
The model is able to predict the initiation of failure.
Numerical simulations useful to understand the mechanics.

The design of structures requires a simple homogenized response.

Homogenization not only important in fiber composites:

- Magnetorheological elastomers
  - Danas et. al (2012)

- Polycrystalline materials
  - Groeber et. al (2008)

- Biological tissue
  - Holzapfel et. al (2001)
Nonlinear homogenization:

Strain energy of heterogeneous materials:

\[
\bar{W}(\bar{F}) = \min_{\bar{F} \in K(\bar{F})} \frac{1}{V} \int_V W(F, X) \, dX
\]

where:

\[
\bar{F} = \frac{1}{V} \int_V F(X) \, dX
\]

Homogenization techniques aim to provide a prediction:

\[
\tilde{W}(\bar{F}) \approx \bar{W}(\bar{F})
\]

Normally expressed as a function of the deformation invariants:

\[
\tilde{W}(I_1, I_2, I_3, I_4, I_5) \approx \bar{W}(\bar{F})
\]

Several predictions exist, with explicit solutions for Neo-Hookean composites.
Iterative homogenization:

\[
\tilde{W}_{IH} = \frac{\tilde{\mu}_{IH}}{2} (\tilde{I}_1 - 3) + \frac{\tilde{\mu}_n - \tilde{\mu}_{IH}}{2} \left(\frac{2}{\sqrt{\tilde{I}_4}} - 3\right) + \frac{\tilde{\mu}_n - \tilde{\mu}_{HS}}{2} \tilde{I}_4
\]

Sequentially coated composites:

\[
\tilde{W}_{SCC} = \tilde{\mu}_{HS} (\tilde{I}_1 - 3) + \frac{\tilde{\mu}_n - \tilde{\mu}_{HS}}{2} \frac{(\sqrt{\tilde{I}_4} + 2) (\sqrt{\tilde{I}_4} - 1)}{\sqrt{\tilde{I}_4}}^2
\]

\[
\tilde{\mu}_n = (1 - V_f) \mu_m + V_f \mu_f
\]

\[
\tilde{\mu}_{HS} = \frac{(1 - V_f) \mu_m + (1 + V_f) \mu_f}{(1 + V_f) \mu_m + (1 - V_f) \mu_f} \mu_m
\]

\[
\tilde{\mu}_{IH} = (1 - V_f)^2 \left(1 + \frac{2 (2 - V_f) V_f \mu_f}{(1 - V_f)^2} \frac{\mu_f}{\mu_m} + \frac{\mu_f^2}{\mu_m^2}\right) \frac{\mu_m}{2}
\]

\[
- (1 - V_f)^2 \sqrt{\frac{2}{(1 - V_f)^2} \frac{\mu_f}{\mu_m} + \left(1 + \frac{2 (2 - V_f) V_f \mu_f}{(1 - V_f)^2} \frac{\mu_f}{\mu_m} + \frac{\mu_f^2}{\mu_m^2}\right) \frac{\mu_f - m \mu_m}{2}}
\]
Numerical homogenization for nonlinear general 3D loading.

Combined model for all loadings

\[
\tilde{W} = \frac{\tilde{\mu}_{IH}}{2}(\tilde{I}_1 - 3) + \frac{\tilde{\mu}_n - \tilde{\mu}_{IH}}{2} \left( \frac{2}{\sqrt{\tilde{I}_4}} - 3 \right)
\]

\[
+ \frac{\tilde{\mu}_n - \tilde{\mu}_{HS}}{2} \frac{\tilde{I}_5}{\tilde{I}_4} - \frac{\tilde{\mu}_{IH} - \tilde{\mu}_{HS}}{2} \frac{\tilde{I}_5}{\tilde{I}_4}
\]

FLJ, Composites B, 2014
PATTERN FORMATION IN SOFT SOLIDS

Collaboration with:

Prof. Pedro Reis (MIT)
Prof. Jorn Dunkel (MIT, Mathematics)
Dr. Romain Lagrange (MIT, Mathematics)
Dr. Norbert Stoop (MIT, Mathematics)
Dr. Denis Terwagne (Universite Libre de Bruxelles)
MOTIVATION AND BACKGROUND

A thin film on a soft elastic foundation wrinkles under compression:

\[ \lambda = \left( \frac{2\pi}{3^{1/3}} \right) h \left( \frac{E_f}{E_s} \right)^{1/3} \]

\[ \sigma_0^C = \frac{3^{2/3}}{4} E_f^{1/3} E_s^{2/3} \]

Allen (1969)

Biaxial compression:

Energy minimization:

Observed experimentally:

Bowden et al. (1998)

Audoly and Boudaoud (2008), Cai et al. (2011)
Drag reduction:

Effect of curvature on wrinkling:

Terwagne et al. (2014)

Lagrange, FLJ, Terwagne, Brojan, Reis (JMPS, in review)
Collaboration with Norbert Stoop and Jorn Dunkel (MIT Math)

The energy minimization in the film can be rewritten as a modified Swift-Hohenberg equation:

\[
\partial_t u = \gamma_0 \Delta u - \gamma_2 \Delta^2 u - au - bu^2 - cu^3 + (\Gamma_1 + \Gamma_2 u) \cdot [ (\nabla u)^2 + 2u \Delta u ]
\]

- stretching
- bending
- local film and substrate
- higher order stretching

Goal:

Treat dimples as lattice elements.

Study the effect of curvature on crystal structures.

Crystallography shown to be independent of the physical potential (Bowick et al., 2002; Bausch et al., 2003)
Planar crystals tend to arrange in regular lattices.

A hexagonal lattice is space-filling and usually minimizes energy.

This is not true in 2D crystals in 3D curved surfaces, where defects are necessary.

Some examples:

- Geodesic dome
- Graphene (Zhang et al., 2014)
- Rotavirus
- Football
- Microcapsules (Chen et al., 2015)
- Colloids (Irvine at al., 2010)
First, there is a topological need:

Topological charge:

\[ s_i = 6 - Z \]

\[ s = 2 \quad s = 1 \quad s = 0 \quad s = -1 \quad s = -2 \]

Euler’s rule:

\[ \chi = E - V - F \]

Total charge:

\[ Q = \sum_i s_i = 6\chi \]

Sphere: \( \chi = 2 \rightarrow Q = 12 \)

Torus: \( \chi = 0 \rightarrow Q = 0 \)

In a sphere that usually means 12 pentagons:

Dodgson (1996)
Second, defects reduce energy required to conform to surface:

As size increases, more defects appear:

Irvine et al, 2012
EFFECT OF SYSTEM SIZE

Similar scaling for all geometries

Agreement with results for colloids:

Bausch et al. (2003)
EFFECT OF CURVATURE

Relationship between defects and curvature:

Gauss-Bonnet: \[ \int K \, dA = 2\pi \chi \]

Euler: \[ \sum_i s_i = 6\chi \]

\[ \int K \, dA = \frac{\pi}{3} \sum_i s_i \]

If we consider larger caps of each solid:
DEFECTS IN ELLIPSOID

Chains:
- Position of centroids
- $\alpha$: Angle between end-to-end vector and tangent $\mathbf{t}$

Single defects

Defect chains

Parallel to equator
Along poles
DEFECTS IN TORUS

Chains:
- Position of centroids
- $\alpha$: Angle between end-to-end vector and tangent $\mathbf{t}$

Single defects

Defect chains

Along $R$ (or $\theta$)
Along $r$ (or $\phi$)
GLOBAL STRUCTURE IN TORUS

Location and structure of defects
Positive: □ □ □ □ □ □ □ □
Negative: □ □ □ □ □ □ □ □

Positive chains: Approximately eight, equidistant, along outer side.

Negative chains: Same number, inner side.

Neutral chains: Between pairs of charged chains, in regions with zero gaussian curvature, perpendicular alignment.

Arrangement of chains can be interpreted as charged particles in an electric field. (Bowick et al., 2004)
GLOBAL STRUCTURE IN TORUS

PDF of distance between centroid of chains shows alignment.

Positive to positive: \( \Delta \theta = \pi/4 \)

Negative to positive: \( \Delta \theta = 0 \).

Neutral to positive: \( \Delta \theta = \pi/8 \).
Global orientation of the crystal lattice:

Hypothesis:
The nucleation of regular (hexagonal) lattice is favored along lines with minimum Gaussian curvature.
PRE-STRETCH INDUCED PATTERNS

New method to create different patterns:

VPS8 – $E \approx 0.22$ MPa

$\lambda_x = \lambda_y \approx 2$

VPS32 – $E \approx 1.2$ MPa

Thickness $\approx 300$ μm
New method to create different patterns:
PRE-STRETCH INDUCED PATTERNS

The ridges are fully bonded.

Different from telephone chord instability.
Test with same material as substrate and thin film.

The wrinkles appear even with no stiffness mismatch.
PRE-STRETCH INDUCED PATTERNS

Self-organized patterns:

Model to study patterns in biological systems:

Pres-stretch & Differential growth

Extend known phase-diagram to biaxial loading:

Applications:

Microfluidics (Moon et al., 2009)
Cellular adhesion (Craighead et al., 2001)
Folding pattern (Tachi, 2015)
Micro lenses (Chand and Crosby, 2006)
MATERIALS FOR OPTICAL ATTENUATION

Optical attenuation changes as the system is stretched:

MATERIALS FOR OPTICAL ATTENUATION

Attenuation as function of stretch:

Beer-Lambert law: \( T = 10^{-\varepsilon c t} \)

3D elasticity: \( t = t_0 \lambda \)

\( T = T_0^{-\lambda} \)

Repeatable and fast:

Predictable:
MATERIALS FOR OPTICAL ATTENUATION

Color dye for band-pass behavior:

Surface topography to increase effect:
SUMMARY AND PERSPECTIVE

Materials with engineered microstructure  +  Nonlinear mechanics of soft and flexible structures

Overall strategy:
Combination of experiments with analytical and numerical work.
Simplified experiments → Modeling → Realistic experiments
Flexible composites

Fiber microbuckling allows high curvatures

Nonlinear behavior and strain softening

Predict failure of fibers in the appropriate geometry

Real fiber microstructure

Response depends on deformation mode
Patterns on soft solids

Curvature influences wrinkling patterns

Model used to study the effect of Gaussian and principal curvatures

Curvature gradient controls defects

New patterns available through pre-stretching

Material for tunable opacity
Engineered microstructure + Soft and flexible structures

Fundamental problems:

- Instabilities
- Failure/damage
- Microstructure
- Homogenization
- Patterns
- Actuation

Applications:

Deployable structures
- Maqueda et al. (2012)

Draping of textiles
- amtcopolis

Soft robotics
- Whitesides group

Solar sails
- University of Surrey

Biomedical devices
- Patterson et al. (2012)

Active mirrors
- Beningo et al. (2002)

Cell characterization
- Rogers et al. (2010)

Flexible electronics

THANK YOU

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- MIT and Masdar Institute Cooperative Program
BACK UP SLIDES
Slight initial curvature may play an important role in mode selection. Can we model its effect?
DEFECTS IN GRANULAR CRYSTALS

Time evolution of defect under horizontal vibration

Defect ~ 450-500 particles
Imaging ~ 0.7 Hz Video 25x speed
f = 28 Hz A = 0.23 mm a = 30 m/s²

Horizontal tray (147x147 mm)
9400 monodisperse brass spheres
d = 1.5875 ± 0.0025 mm (1/16” grade 200)
DEFECTS IN GRANULAR CRYSTALS

Crystal – Defect – Boundary

Structure on boundary correlates with misorientation:

- High (25-30°)
- Medium (15-20°)
- Low (5-10°)

Coincident lattice
Glassy region
Dislocations

Local Voronoi density:

- Crystal
- Defect
- Boundary

Voronoi density (\( \phi \))

Pdf

0.6 0.7 0.8 0.9 1
DEFECTS IN GRANULAR CRYSTALS

High spread in healing time.

Next step: high speed camera to measure “temperature”.

\[
T = T_0 e^{k\alpha}
\]

\[
k = -0.24 \pm 0.04 \quad [1/\text{deg}]
\]

\[
T_0 = 1295^{+732}_{-467} \quad [\text{s}]
\]

Goal:
Model system to study the dynamics of grain boundaries in general crystalline media.
Implicit assumption: isotropy of the RVE.

Is the response the same for all loading directions?

Principal stretches:

Incompressibility:

Plane strain:

Spectral theorem:

All deformations can be described by stretch and direction:

\[
\begin{align*}
\lambda_1 &= \lambda \\
\lambda_2 &= 1 \\
\lambda_3 &= 1/\lambda \\
n_1 &= [0 \quad \cos \theta \quad \sin \theta] \\
n_2 &= [1 \quad 0 \quad 0] \\
n_3 &= [0 \quad -\sin \theta \quad \cos \theta]
\end{align*}
\]
Ten different realizations of the RVE.

Response is a sine:

\[ \mu_\theta = \tilde{\mu} + \Delta \mu \sin (4\theta + \theta_0) \]

Parameters change for each RVE.

Expected value:  \[ E_{RVE}[\tilde{\mu}_\theta] \]

Coefficient of variation:  \[ CV_{RVE}[\tilde{\mu}_\theta] = STD_{RVE}[\tilde{\mu}_\theta]/E_{RVE}[\tilde{\mu}_\theta] \]
HOMOGENIZATION

Considering all directions reduces variability between models and improves convergence in response.

\[ \delta = \frac{L}{R} \]

FLJ, Composites B, 2016
Fiber-matrix interphase
(with Prof. Lopez-Pamies)

Effect of thin layer of material between fiber and matrix.

Homogenized response including damage

Introduce strain softening and damage into homogenized response.

Numerically efficient homogenization

Reduce the cost of numerical homogenization, taking into account:
• RVE anisotropy
• Range of fiber interaction.