Multi-Physics Modeling of Environmentally-Activated Network Polymers

SAND2011-5748P

Sandia National Laboratories

Kevin N. Long, SNL NM
Professors Martin Dunn and H. Jerry Qi, Dept. Mechanical Engineering, University of Colorado, Boulder

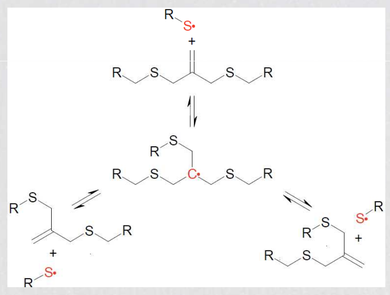
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Early Career R&D Program

Problem

How do we take advantage of this behavior…

Molecular Mechanism:

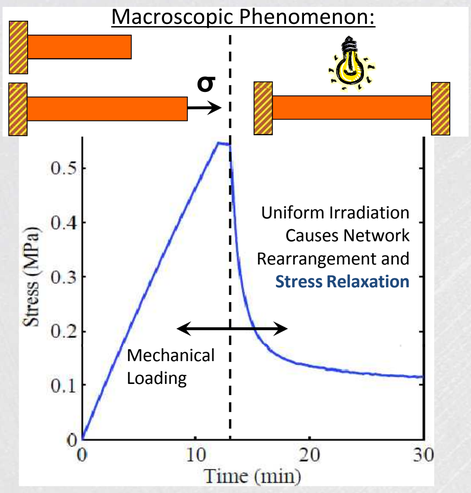


radicals undergo addition/ fragmentation chain transfer reactions at C=C sites

*** **Network Connectivity Rearranged*****

R Denotes Chain Continuation

Macroscopic Phenomenon:



…to produce adaptive structures, sensors, and healing materials?

Main Objective: Develop experimentally validated, mechanistically-driven material models for photo and thermally responsive network polymers for use in sensing, actuation, and encapsulation applications.

Approach

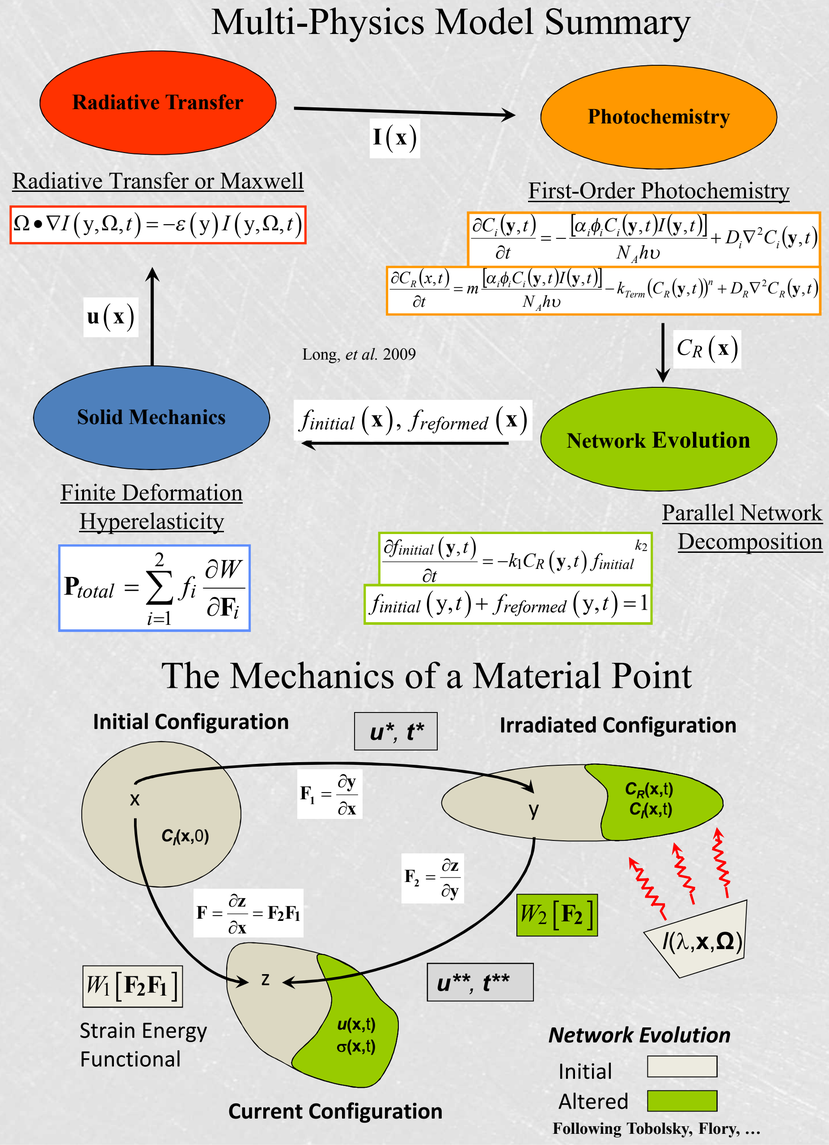
Modeling such materials requires expertise and efforts from multiple disciplines which makes this project well suited for a national laboratory. This project has three major components:

Experiments
- Material Characterization and Optimization
- Actuator Realization

Constitutive Modeling
- Couple radiative transfer, photo and/or thermal-chemistry, network evolution, and solid mechanics

Theory and Simulations
- Build Analytic Models of Simple Actuator Designs
- Optimize Actuator Design and Performance with Finite Element Analysis

Multi-Physics Model Summary

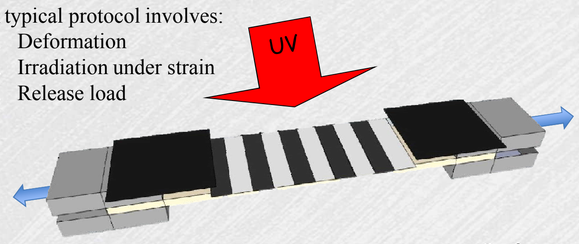


The Mechanics of a Material Point

Results

1D Photo-Mechanical Patterning: Optically Thin Films and Poisson Effects

A typical protocol involves:
1. Deformation
2. Irradiation under strain
3. Release load



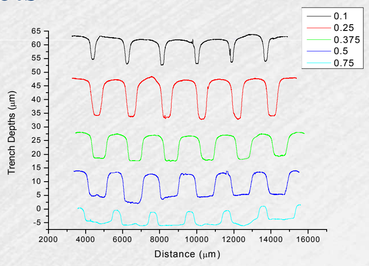
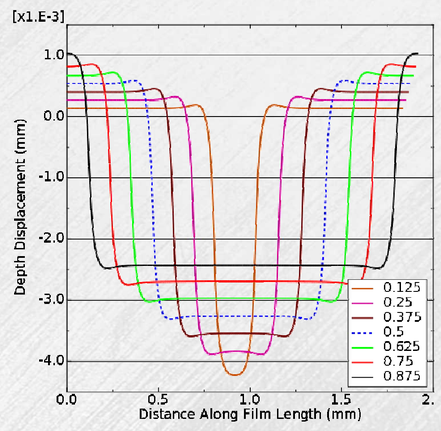
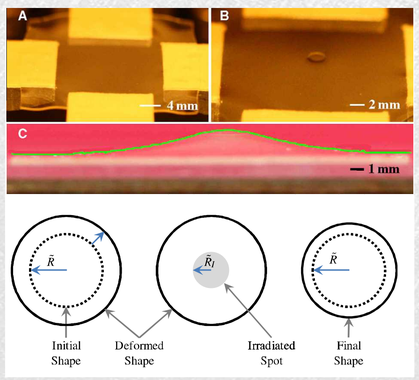


Image of a typical mechanical profilometer scan with trenches visible

Surface profiles for different ratios of the irradiated zone length to the periodic pattern length. Experimental and periodic finite element results are shown above/below.



2D Photo-Mechanical Patterning: Optically Thin Films and Elastic Instabilities



Long, *et al.* 2011

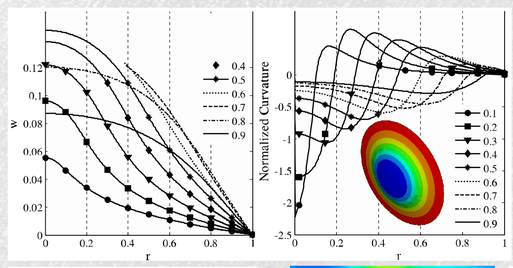
Above: Procedure used in analytical and parametric studies using finite elements.

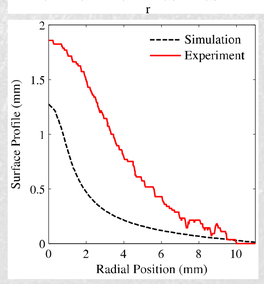
Right: Comparison between finite element calculations and a typical dimple surface.

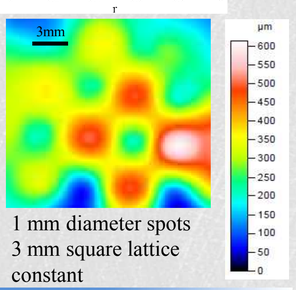
Far Right: Experimental realization of the buckling of a thin film that was uniaxially extended, irradiated with a square array of circular spots, and released.

Left: Experimental realization of controllable dimples via biaxial deformation and relaxation of a circular spot.

Below: finite element parametric study of the dimple curvature and surface profile as it depends on the ratio between the spot radius and diameter of the disk.







1 mm diameter spots
3 mm square lattice constant

Significance

Impact: Environmental-mechanical couplings enable unique "smart" material applications, including:
1.Removable or self-healing encapsulation for electronics packaging
2.Tunable surface patterns for micro fluidics
3.Remotely activated structures such as the box shown on the right, which folded after exposure through a simple photo-pattern at its joints
4.Novel sensors that respond to specific frequencies

Future Work: Efforts of this research are being applied to:
- thermally-removable networks that incorporate Diels-Alder functionalities
- Interpenetrating networks that are individually or collectively photochemically and mechanically responsive

References:

Long, K.N., et al. 2011. Photo-induced deformation of active polymer films: single spot irradiation. I. J. Solids and Structrues

Long, K.N., et al. 2009. Photomechanics of Light-Activated Polymers. J. of the Mechanics and Physics of Solids

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000."

SAND 2010-xxxP

Sandia National Laboratories