Microstructural Design of Light-Induced Phase Transformation Materials

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Background

♦Photomechanical molecular materials have the potential to revolutionize energy conversion technologies. These materials undergo a first-order phase transformation when exposed to light causing them to exhibit various modes of deformations, ranging from simple stretching to exploding into several pieces. In this project, I aim to investigate the fundamental mechanism underpinning three modes of deformations—stretching, bending, and twisting—in photomechanical molecular materials.

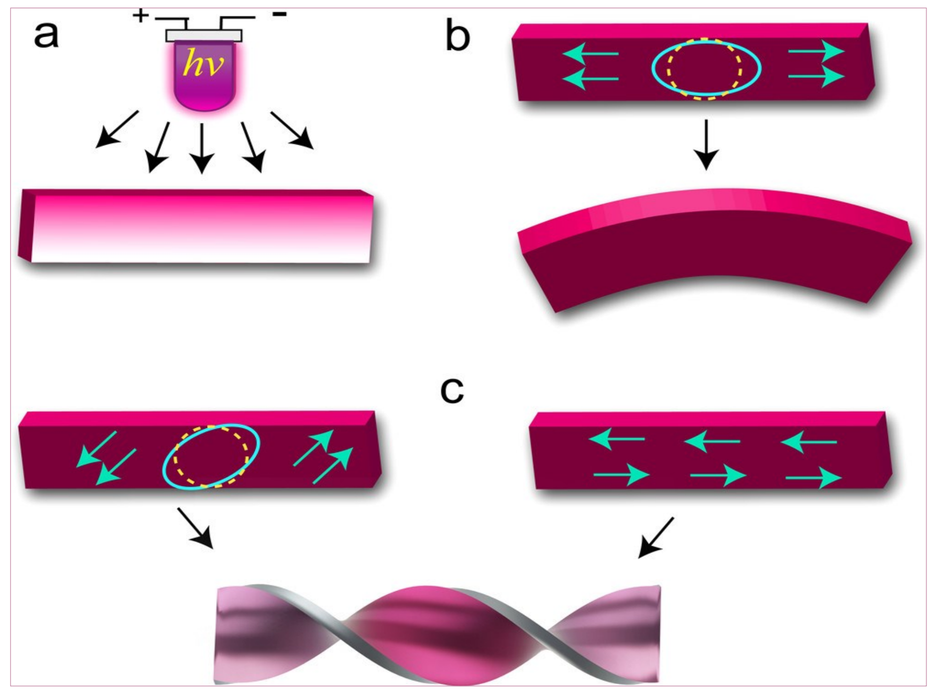


Fig.1 Bending and twisting due to photo-induced phase transformation [1]

♦**Why Light Stimulus?**

♦Contactless actuation and Unique photo-triggered phase transition

♦Controlled deformation modes by changing illumination condition (frequency, intensity, and polarization)

Hypothesis

♦Previous research explained the deformation modes of photomechanical materials by comparing the lattice structure of these materials before and after illumination. This approach, in isolation, does not explain the complex bending or twisting deformations in these materials. We hypothesize that we need to understand the full structural transformation pathway, from the material's initial state to its end state, the microstructural patterns that evolve during this transformation, and how these processes interact with evolving light intensities and material heterogeneities, to predict and control the specific photomechanical response it will exhibit.

Continuum Theory

♦**Cauchy-Born Hypothesis:** In a crystalline solid subject to a small strain, the positions of the atoms within the crystal lattice follow the overall strain of the medium

♦Therefore, local structural phase transformation results in macroscopic deformation

♦Microstructural patterns govern the mode of macroscopic deformation, for instance, bending is commonly observed in microstructures with distinct two-phase pattern

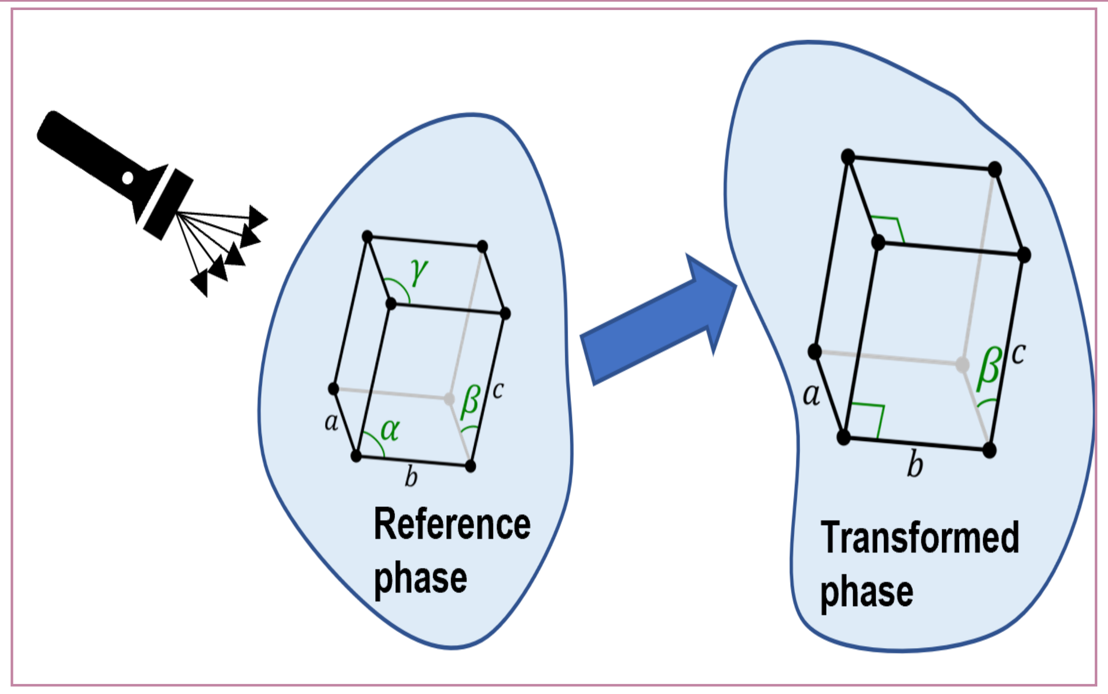
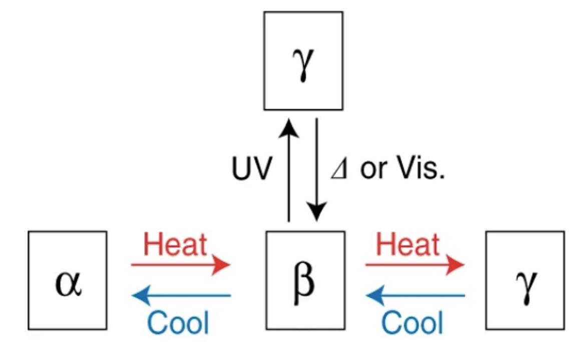


Fig.2 Photo-induced phase transformation

Experimental Observation

♦On exposure to UV radiation, photochromic chiral salicylideneamine crystal undergoes enol-keto photoisomerization accompanied with structural transformation from β(triclinic) to γ(monoclinic) phase



♦The γ phase obtained from photo-triggered phase transition is a unique state and can not be obtained from thermal phase transition [2]

♦Phase change (β-γ) is the reason behind appearance of twist deformation in Fig.3

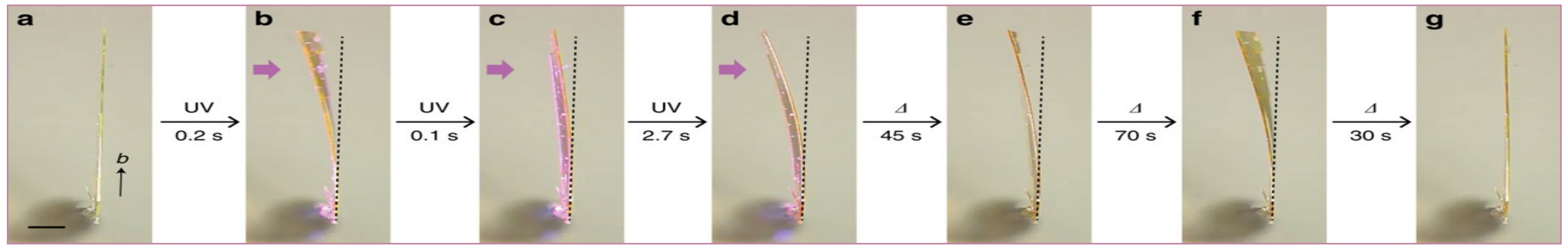


Fig.3 Stepwise Bending of thin plate-like crystal due to light-induced phase transformation [2]

Phenomenological Model

♦**Phase-field model for coupled mechanical deformation and phase transformation**: free energy constitutes elastic energy of deformation and gradient interfacial energy

$$\psi(\mathbf{E},\phi) = \iiint_V [\psi_{elastic}(\mathbf{E},\phi) + \psi_{interface}(\phi,\nabla\phi)]\, dV$$

$$\psi_{elastic} = \frac{1}{2}[\mathbf{E}-\mathbf{E}_0(\phi)] : C[\mathbf{E}-\mathbf{E}_0(\phi)]$$

$$\psi_{interface} = \phi^2(1-\phi^2) + k(\nabla\phi)^2$$

where Φ is a non-conserved order parameter

$$\phi = \begin{cases} 1 & \text{transformed phase}(\gamma \text{ - Monoclinic}) \\ 0 & \text{reference phase}(\beta \text{ - Triclinic}) \end{cases}$$

♦Simulation result: A beam specimen is subjected to flux boundary condition on one face

♦Propagation of phase boundary results in stepwise twist deformation

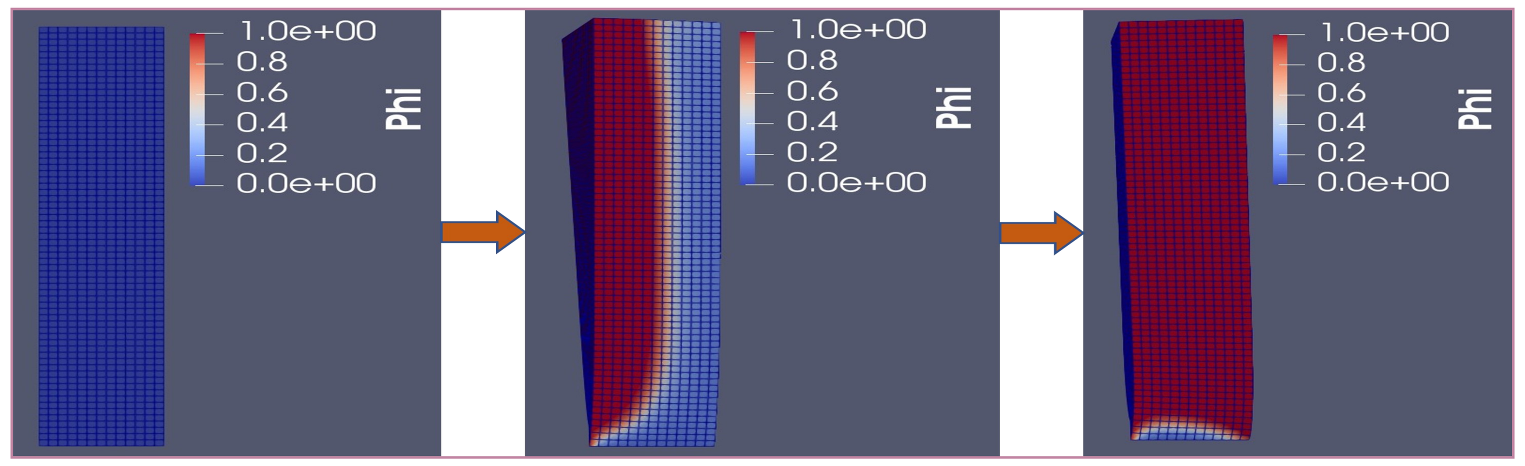


Fig.5 Stepwise deformation with propagation of phase boundary

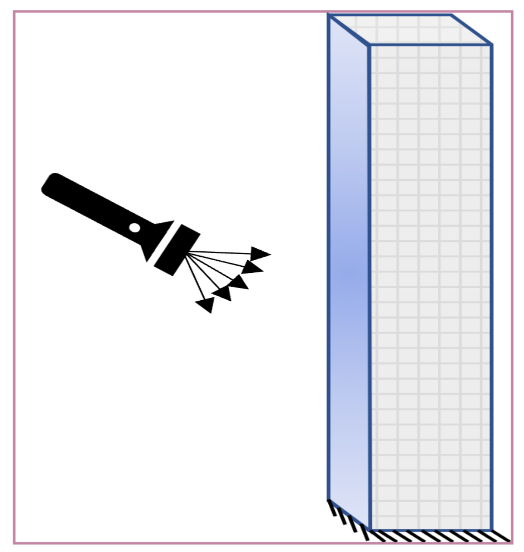


Fig.4 Simulation setup

Future Work

♦To model interplay between incident radiation and finite deformation

♦Tailor microstructural design for targeted deformation pattern

Acknowledgement: *The authors acknowledge the support of an AFOSR YIP award by the US Department of Defence (Materials with Extreme Properties) in carrying out this work.*

[1] Naumov, P., Chizhik, S., Panda, M.K., Nath, N.K. and Boldyreva, E., *Chemical reviews*, **2015**, 115(22), pp.12440-90.

[2] Taniguchi, T., Sato, H., Hagiwara, Y., Asahi, T. and Koshima, H., *Communications Chemistry* , **2019**, 2(1), pp.1-10.