Micromechanics of Dynamic Materials

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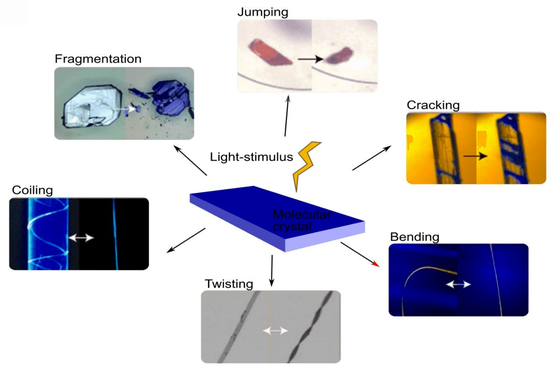
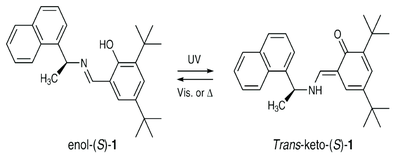
Motivation

- What makes some of these crystals to bend and twist while others to jump and explode when exposed to light?
- In our research, we investigate how underlying structural transformations and microstructural evolution path-ways govern the photomechanical be-havior



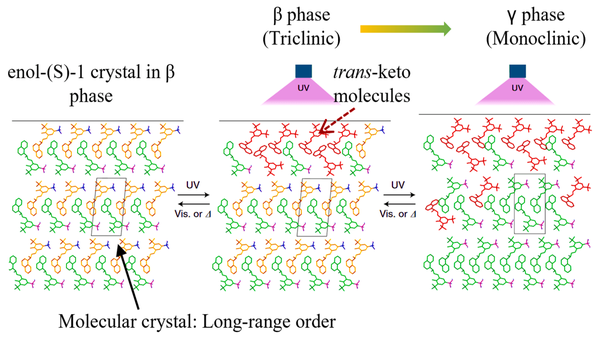
Experimental observation

- Photochromic chiral salicylideneamine crystals undergo enol-keto photoisomerization on ex-posure to UV radiation

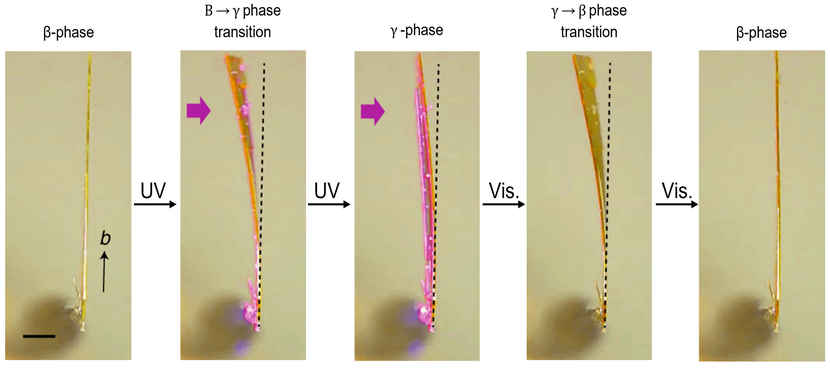


enol-(*S*)-**1** *Trans*-keto-(*S*)-**1**

- This photoisomerization drives a structural transformation from β(monoclinic) to γ(triclinic) phase



- At the macroscopic level, this structural transformation induces a bending-twist deformation



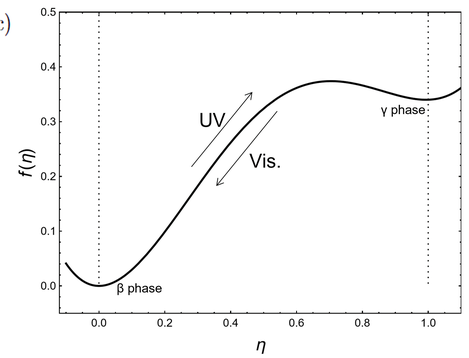
Scan the QR code to see the movie of stepwise bending-twist deformation

Phenomenological Model

- We develop a phase field model—implemented in finite element framework to study macroscopic photo-mechanical deformation based on microstructural evolution
- Non-conserved order parameter $\eta = \begin{cases} 1 & \text{transformed phase}(\gamma \text{ - Monoclinic}) \\ 0 & \text{reference phase}(\beta \text{ - Triclinic}) \end{cases}$
- Total energy of the system

$$\psi = \int_{\mathcal{E}} f(\eta) + \frac{\kappa}{2}|\nabla\eta|^2 + \frac{1}{2}[\mathbf{E} - \mathbf{E}_0(\eta)] : \mathbb{C}[\mathbf{E} - \mathbf{E}_0(\eta)]\mathrm{d}\mathbf{x}$$

Free energy; Interfacial energy; Elastic energy of deformation



Applied UV radiation drives the phase transition drives the phase transition to metastable γ phase

- The order parameter evolves following driven time-dependent Landau-Ginzburg equation

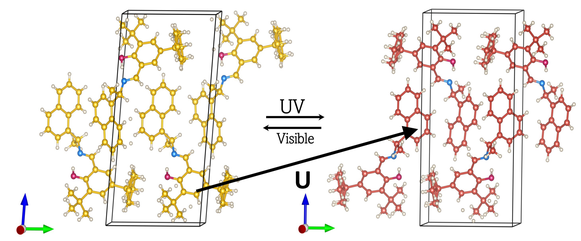
$$\frac{\partial \eta}{\partial t} = -\mathrm{M}_0\left[\frac{\partial f}{\partial \eta} - \nabla.(K\nabla\eta)\right] + \lambda \mathrm{I}(1-\eta)$$

Drives the system to the minimum energy state; Driving force for β- to γ-phase transformation

- State-dependent spontaneous or stress-free strain

$$\mathbf{E}_0(\eta) = \eta(\mathbf{U} - \mathbf{I} + \delta \mathrm{e}^{-\lambda \mathrm{d}}\,\hat{\mathbf{e}}_2 \otimes \hat{\mathbf{e}}_2)$$

β-to-γ phase transformation; Enol-keto photoisomerization



Change in crystal structure due to phase transition (Triclinic - Monoclinic)

Simulation Results

- Interplay between irradiation flux and energy minimization describes the bending and twisting behavior

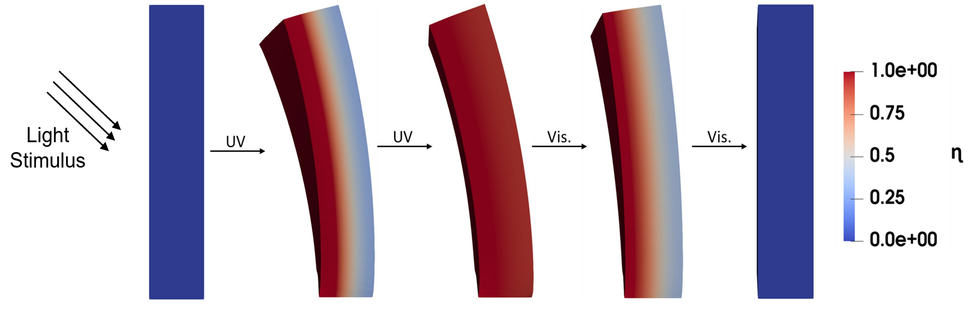


Photo-induced phase transformation induc-ing stepwise bending -twist deformation; (a -c) β-to-γ, (c-e) γ-to-β phase transfor-mation

Acknowledgement

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

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[2] Taniguchi, T. et al., *Communications Chemistry* , **2019**, 2(1), pp.1-10

[3] Tiwari D., Balakrishna A.R., 2023 (manuscript in preparation)