

# **I** Mechanically-driven Nano-manufacturing of Atomically-thin Origami and Kirigami Structures



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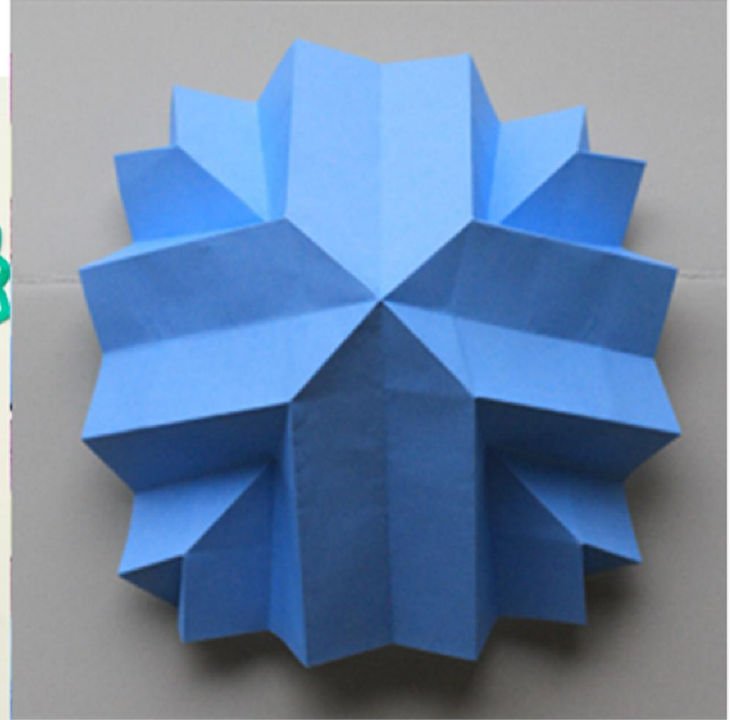


**Mechanics of  
Materials**  
-Straining  
-Deformation

**Material  
Properties**

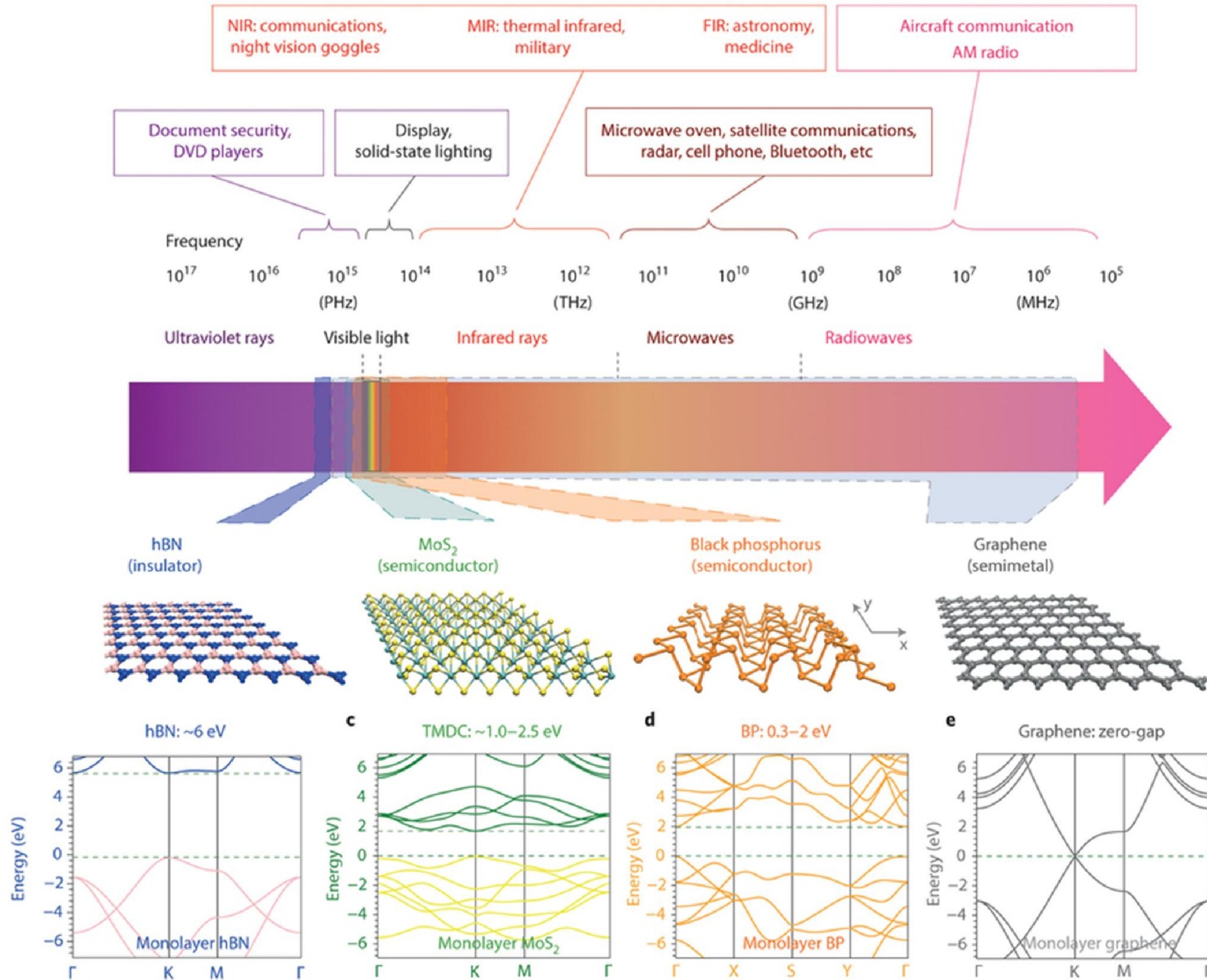
- Thermal
- Chemical
- Electrical/Optical





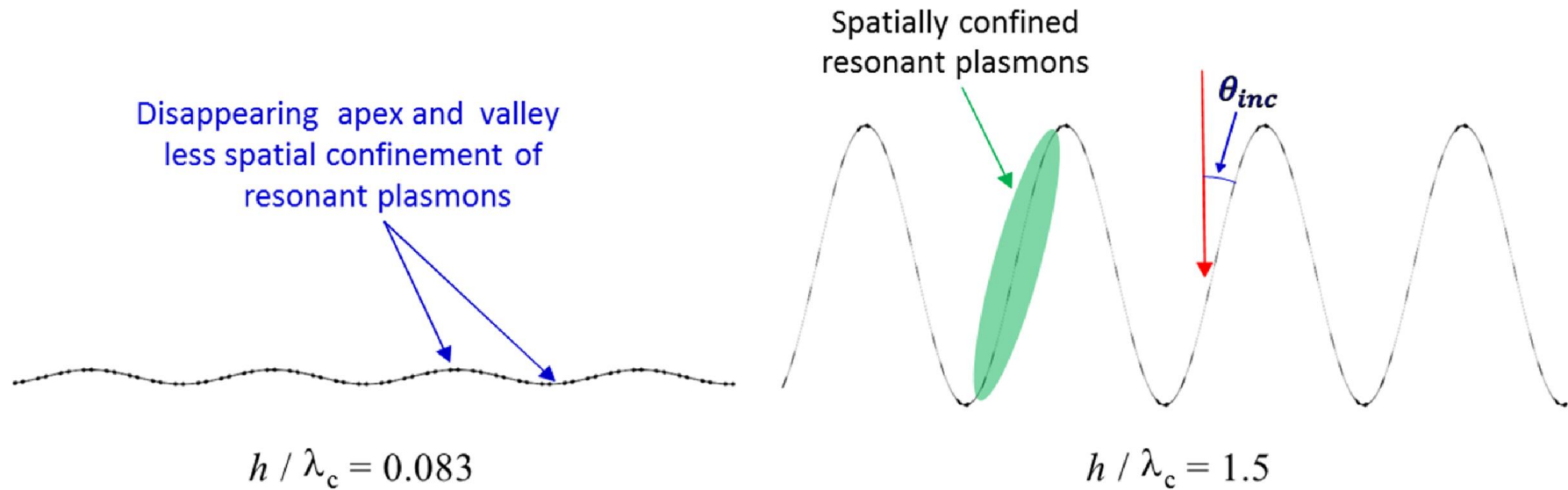


# Atomically-thin, 2D Materials





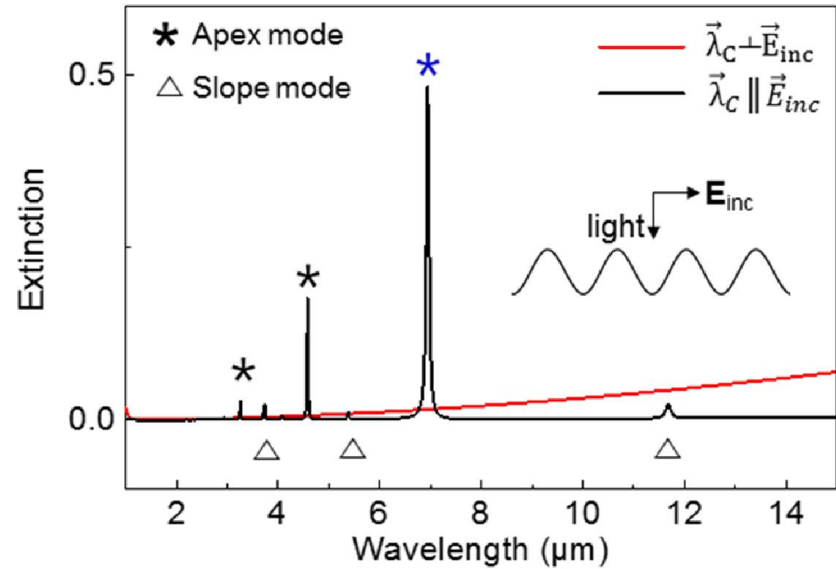
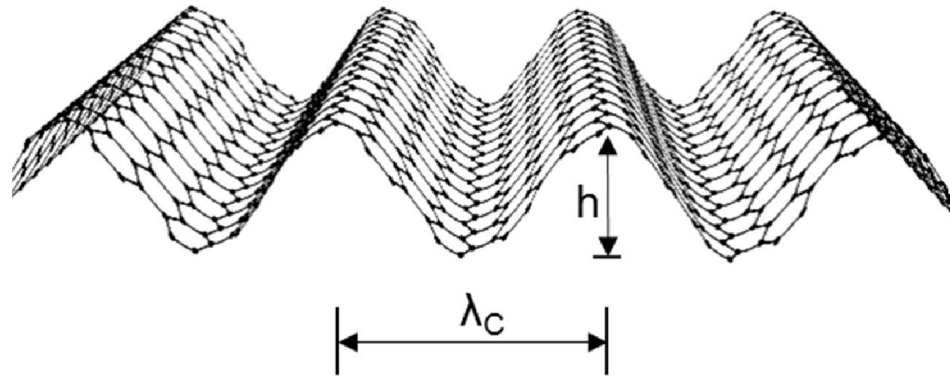
# Topography vs. Plasmons



- Crumpling graphene enables the enhanced plasmonic resonance in the near/mid infrared wavelengths (1-10  $\mu\text{m}$ ) which is difficult to achieve with the lithographically patterned graphene nanostructures (e.g. graphene ribbons, disks, rings, and stacks).
- Stretching/releasing of crumpled graphene enables new possibilities of reconfigurable graphene plasmonics (meta-materials).



# Topography vs. Plasmons



Random phase approximation method used.  
The optical conductivity of graphene is given by

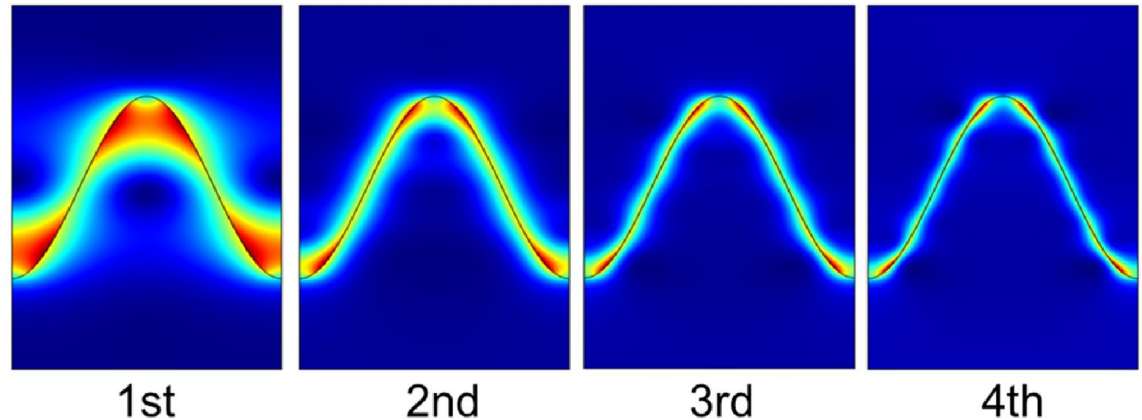
$$\sigma(\omega) = \sigma_{intra}(\omega) + \sigma_{inter}(\omega)$$

$$\sigma_{intra}(\omega) = \frac{2e^2\omega_T}{\pi\hbar} \frac{i}{\omega + i\tau^{-1}} \log \left[ 2 \cosh \left( \frac{\omega_F}{2\omega_T} \right) \right]$$

$$\sigma_{inter}(\omega) = \frac{e^2}{4\hbar} \left[ H \left( \frac{\omega}{2} \right) + i \frac{2\omega}{\pi} \int_0^\infty \frac{H \left( \frac{\omega'}{2} \right) - H \left( \frac{\omega}{2} \right)}{\omega^2 - \omega'^2} d\omega' \right]$$

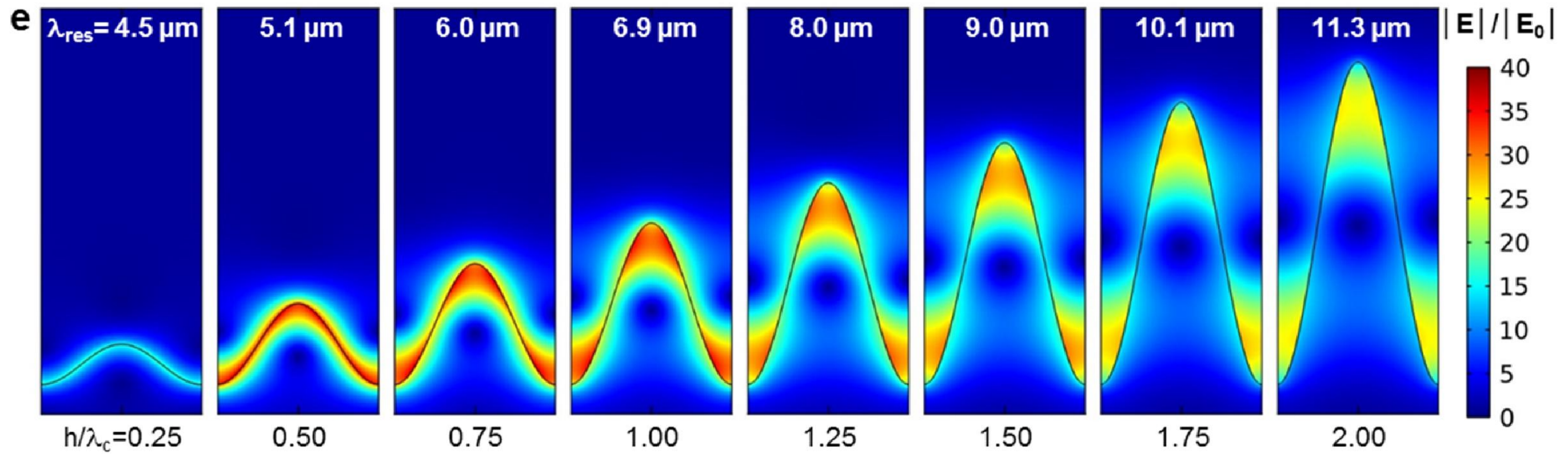
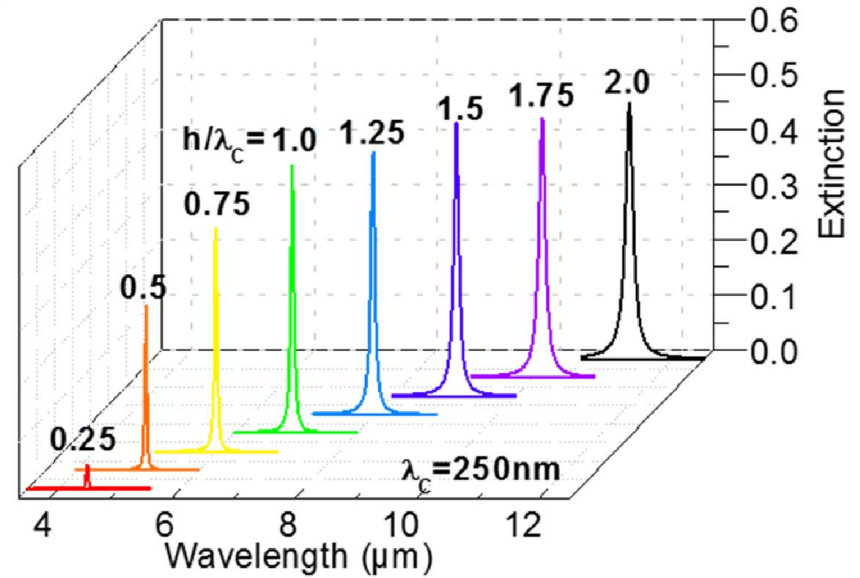
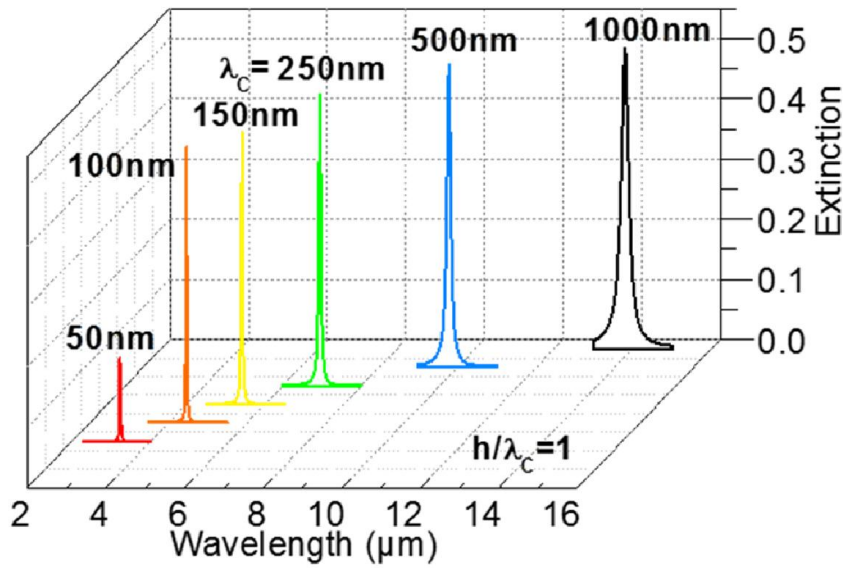
$$H(\omega) = \frac{\sinh(\omega/\omega_T)}{\cosh(\omega_F/\omega_T) + \cosh(\omega/\omega_T)}$$

$$\omega_F = E_F/\hbar, \quad \omega_T = k_B T/\hbar, \quad \hbar = \frac{h}{2\pi}$$





# Topography vs. Plasmons



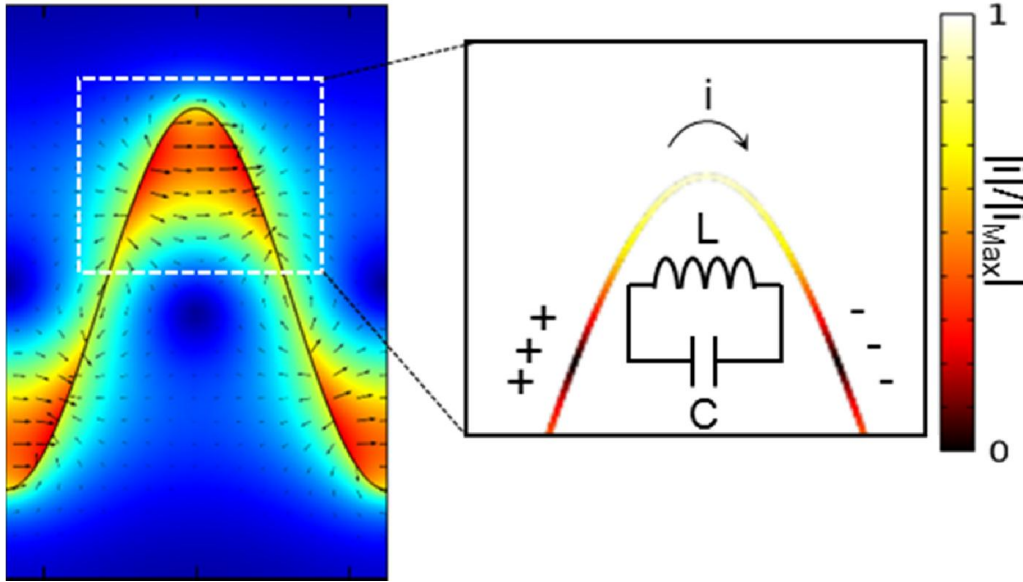


# Topography vs. Plasmons

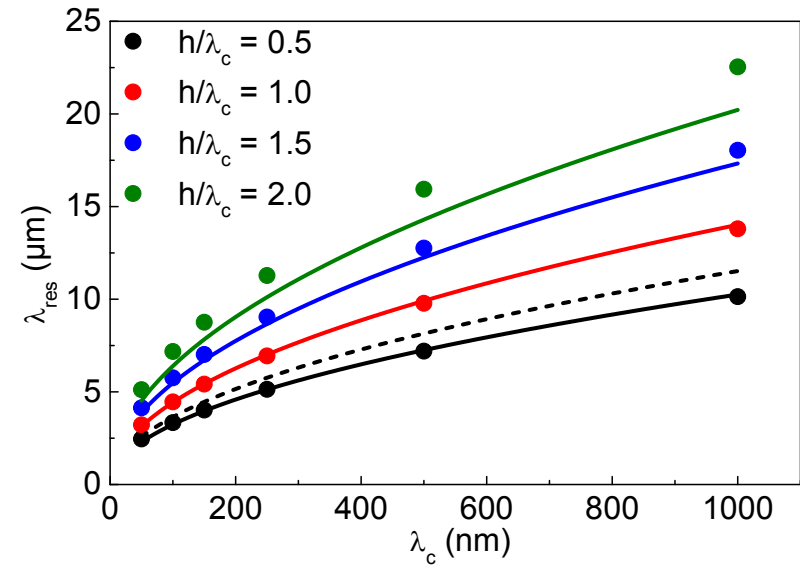


**Mechanically Reconfigurable  
Architected Graphene Metamaterial  
for  
Broadband Tunable  
Plasmonic Resonances**





Conventional Model



New LC-circuit Model

$$\lambda_{res} = 2\pi c \sqrt{\frac{\hbar^2 \varepsilon_0 (\varepsilon_1 + \varepsilon_2)}{e^2 E_F} \frac{\lambda_c}{2}}$$

Our analytical model accurately describes the surface plasmon resonance of crumpled graphene with small to large  $h/\lambda_c$  (0.2–2).

$$\lambda_{res} = 2\pi c \sqrt{L_{eff} C_{eff}}$$

$$L_{eff} = \frac{\pi \hbar^2}{e^2 E_F} \lambda_c$$

$$C_{eff} = \varepsilon_0 \left( \frac{\varepsilon_1 \varepsilon_2}{\varepsilon_1 + \varepsilon_2} \right) \frac{1}{\alpha} \ln \left[ 1 + (1 + e^{-\alpha}) \right]$$

$$\alpha = \pi - 2 \tan^{-1} (2h/\lambda_c)$$



# Mechanically-driven Nano-manufacturing of Ultrathin Kirigami Structures



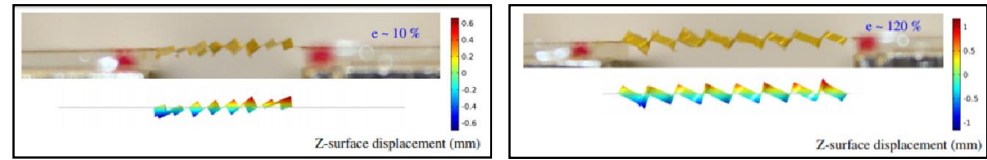
**nanoMFG node thrust:**  
VI Nanoscale Self Assembly

**PIs and Students:** Aluru & Nam (PIs);  
De & Yong (students)

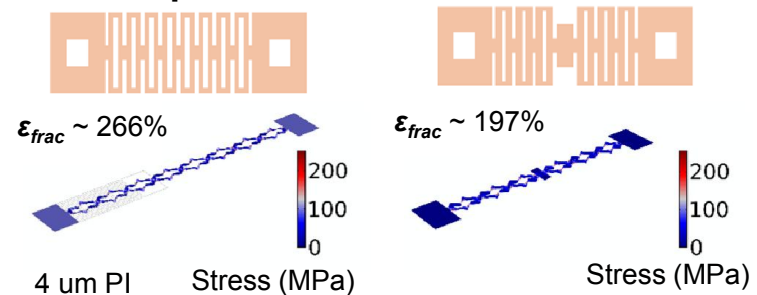
**Objectives:** Develop a simulation tool capable of nano-mechanics driven manufacturing of ultrathin kirigami structures for meta materials.

- (1) Develop continuum mechanics model for several deformation modes
- (2) Experimental verification of final structures

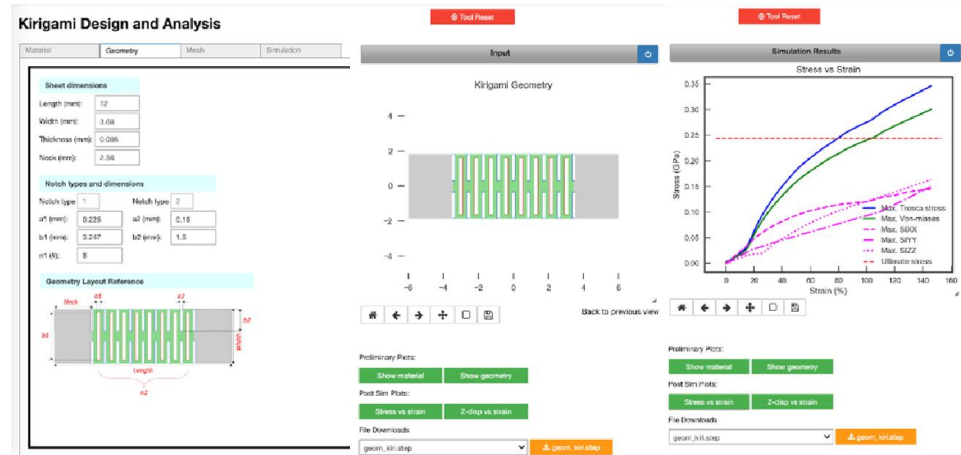
**Significance:**  
Use mechanical self-assembly to create multifunctional structures and morphologies in nanoscale



## Experiment vs. Simulation



## Parametric Optimization



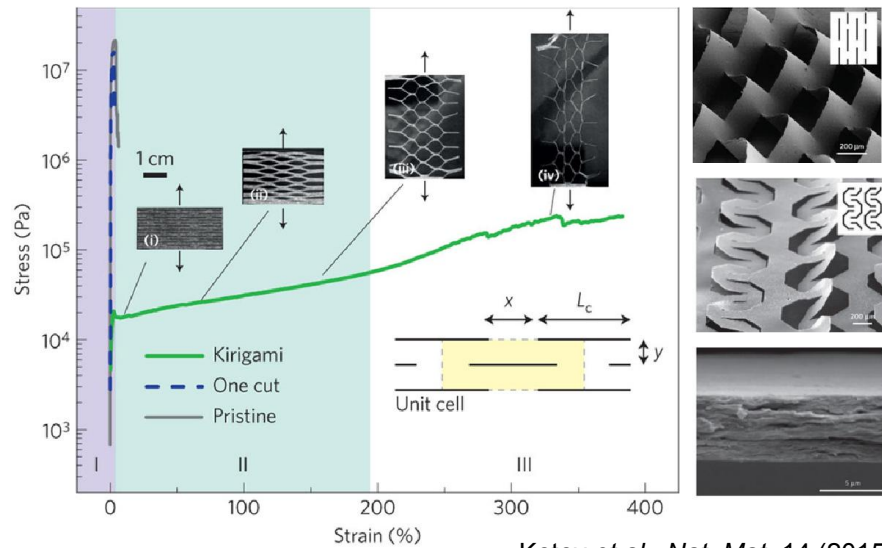
## Tool Wireframe



# Inspirations for Kirigami Architecture

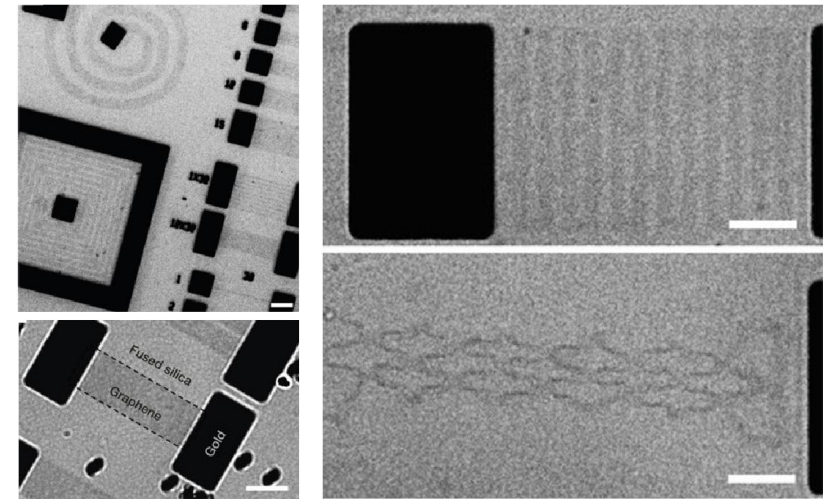


## Kirigami Paper/Nanocomposite



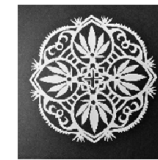
Kotov et al., *Nat. Mat.*, 14 (2015)

## Graphene Kirigami



McEuen et al., *Nature.*, 524 (2015)

- In traditional kirigami, cut or notches are introduced into paper sheets to attain a desirable topology on folding.
- 2D kirigami surface architectures can be transformed into strain-responsive 3D architectures in the vicinity of patterned regions owing to mechanical bi-stability.





# nanoHUB Tool Interface (1)



## Kirigami Design and Analysis

Material | Geometry | Mesh | Simulation

**Material Properties**

Select material: polyimide

Material name: polyimide

Poisson's ratio: 0.34

Density (kg/m3): 1420

Young's Modulus (GPa): 2.1

**Traction Analysis\***

Yield strength (GPa): 0.103

Ultimate stress (GPa): 0.244

\*The traction curve is an experimental point by point curve of stress vs. strain generated from monotone traction testing for the given material. The traction curve should start from  $(R_{p0.2}/E, R_{p0.2})$  and go to the breaking point, where  $R_{p0.2}$  is the offset yield point and E is Young's modulus in Gpa.

Tool Reset

Input

polyimide - Stress vs Strain

Stress (GPa)

Strain (%)

— Before yield

○ After yield

- - - Ultimate stress

Home | Back | Forward | Zoom In | Zoom Out | Save

Preliminary Plots:

Show material | Show geometry

Post Sim Plots:

Stress vs strain | Z-disp vs strain

File Downloads

geom\_kiri.step | geom\_kiri.step

<https://nanohub.org/tools/gamian>



# nanoHUB Tool Interface (2)



## Kirigami Design and Analysis

Material | **Geometry** | Mesh | Simulation

**Sheet dimensions**

Length (mm):

Width (mm):

Thickness (mm):

Neck (mm):

**Notch types and dimensions**

Notch type     Notch type

a1 (mm):     a2 (mm):

b1 (mm):     b2 (mm):

n1 (#):

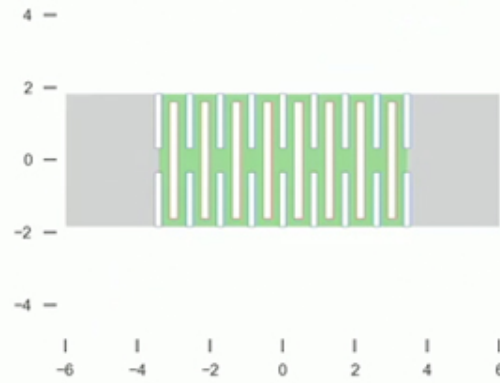
**Geometry Layout Reference**

The diagram shows a rectangular sheet with a central region containing a series of vertical notches. The notches are labeled 'a1' and 'a2'. The central region is labeled 'Length' and 'n1'. The left and right ends are labeled 'Neck'. The total height is labeled 'Width' and 'b1', and the height of the notched region is labeled 'b2'.

⊕ Tool Reset

Input

Kirigami Geometry



Back to previous view

Preliminary Plots:

Post Sim Plots:

File Downloads

<https://nanohub.org/tools/gamian>



# nanoHUB Tool Interface (3)



## Kirigami Design and Analysis

Material | Geometry | **Mesh** | Simulation

**Sizing control**

No. of segments along the thickness:

Max. 2D mesh size :

**Mesh stats**

No. of nodes: 3508  
No. of elements: 10702

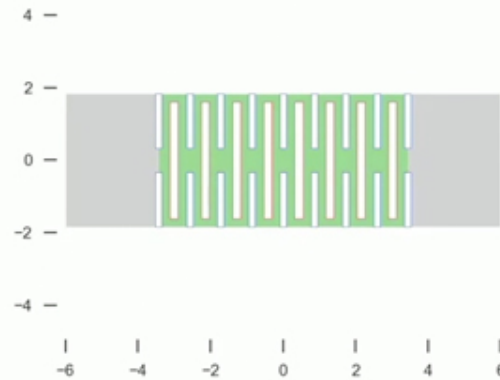
To visualize the geometry and mesh, download the mesh\_kiri.med from File Downloads and use paravis module in the Salome software suite

Output

Last Run: OK. Run Time: 00:00:12

Input

Kirigami Geometry



Preliminary Plots:

Post Sim Plots:

File Downloads

<https://nanohub.org/tools/gamian>



# nanoHUB Tool Interface (4)



## Kirigami Design and Analysis

Material | Geometry | Mesh | Simulation

**Perturbation force**      **Stretching**

Final value (Newton):       Final value (mm):

No. of steps:       No. of steps:

**Solution storing**

Store solution every 'Nsto' steps:

**Convergence**

1st level step cutting:

2nd level step cutting:

Max iter/time step:

Rel residual:

Abs residual:

Tan matrix reval every 'mf' time increments:

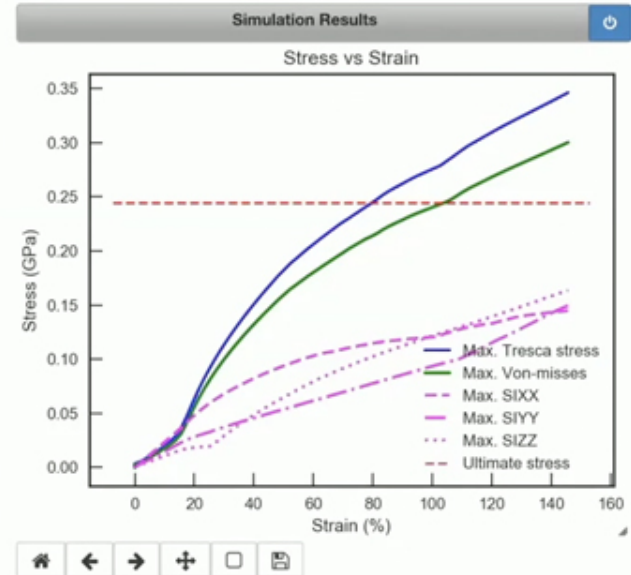
Tan matrix reval every 'it' Newton iterations:

tractionConv.csv... Found

mesh\_kiri.med... Found

Output

Last Run: OK. Run Time: 00:06:03



Preliminary Plots:

Post Sim Plots:

File Downloads

geom\_kiri.step

<https://nanohub.org/tools/gamian>



# Conclusions



- **Controlled Deformation for**
  - Reconfigurable plasmonic resonance of corrugated graphene
- **Kirigami Design for**
  - Decoupling mechanical response from electrical properties of the design structure
- **Acknowledgements:** nanoMFG, NSF CMMI, i-MRSEC/DMR

