Supplementary material – Kirigami Actuators

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Methods Section

Fabrication: Mylar (BoPET) films were purchased from McMaster–Carr (Mylar, 8567K96), and had a thickness of $h = 0.127$ mm. To relieve any residual stress in the films, apparent from their natural curvature, we annealed the films in the oven at 85^oC under the weight of thick metal sheets for 2 hours, resulting in flat sheets. Vector patterns were drawn in Adobe Illustrator CS6, and cut with an Epilog Mini 24, 75W laser cutter in vector mode, at 80% speed and 10% power. Sheet widths of $w = 40$mm, 60mm, 80mm, and 100mm were used, and sheet lengths of $L = 20$mm to 200mm in linear increments of 20mm were used. For the single cut experiments, cut lengths ranging from $b = 20$mm to 70mm were used. The cut mylar films were adhered to 3mm thick acrylic sheets (McMaster–Carr, acrylic, 8560K191) with cyanoacrylate glue (McMaster-Carr, Loctite 403, 74765A53), which served as the clamped boundary conditions for the films.

Mechanical Measurements: Uniaxial tension tests were performed by clamping the mylar sheets to the Instron 5943 mechanical testing system, using a 500N load cell. Displacement–controlled tests were performed at a rate of 0.15mm/min to a maximum extension of 1.5mm. Since the mylar did not experience inelastic strains, actuation was reversible, and 3 tests were run for each sample. Actuator deformation was captured from the side with a microscopic lens (Navitar Zoom 6000) attached to a Nikon D610 camera, and from the front using a Nikon D610 camera with a Micro-NIKKOR 105mm f/2.8 Lens, a Nikon 55mm f/2.8 Lens, and a high contrast Rosco Color Filter (B&H Photo Video, ROCEK1212). The critical buckling force was determined from identifying both the slope change in the force vs. displacement curve, and the out–of–plane deflection from the microscopic imaging of the crack profile.

Finite Element Method (FEM): FEM simulations were undertaken using COMSOL Multiphysics 5.2[1] along with the Structural Mechanics Module. Shell Mechanics and Plates were the environments within COMSOL in which all of our studies were performed. A geometry matching those used in the experiment was created in COMSOL's Design Module. Mesh refinement studies were undertaken to ensure convergence of the results. For the single cut geometry in figure 2, the sheet was modeled as an isotropic elastic thin sheet with thickness of $h = 0.127$mm, Young's Modulus $E = 3.5$GPa, and Poisson's ratio $\nu = 0.38$. The results shown in figure 2*c* were attained through linear buckling studies with varying thickness in the range $h \in [0.1\text{mm}, 0.14\text{mm}]$ and

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the values $b/w \in [0.3, 0.8]$. The in–plane results shown in figure 2*a* and post-buckling results in figures 2*d*, 3, and 4 were calculated from a stationary study with displacement (Δ) controlled analysis. In order to induce out–of–plane symmetry breaking, we added random small imperfections (ten orders of magnitude smaller than the sheet thickness) to the initial surface. The parameters in figure 2*d* varied and lay in the ranges $h \in [0.15\text{mm}, 0.21\text{mm}]$ and $b/w \in [0.1, 0.9]$. For the results shown in figure 5, linear buckling studies were undertaken with the boundary at $x = 0$ fixed in space while the boundary at $x = L$ had an imposed displacement of Δ in the x direction. Both of these boundaries were not permitted to rotate. All other boundaries were free. Small imperfections in the form of the first eigenmodes were then added to the initially flat geometry through use of MeshPerturb 1.0[2]. These imperfect geometries were then used for the stationary studies with the same boundary conditions and the same mesh density as was used in the linear studies.

Molecular Simulations: We used Sandia-developed open source LAMMPS Molecular Dynamics Simulator to simulate graphene sheets[3]. To describe the carbon-carbon interactions, we used AIREBO potential[4] as has been used previously in atomistic study of graphene kirigami[5]. The cutoffs for the Lennard-Jones and the REBO term in AIREBO potential are chosen to be 2 Å and 6.8 Å, respectively. For MoS_2 actuators we used the Stillinger-Weber potential developed by Jiang[6], which we have previously employed to study MoS_2 kirigami[7]. Graphene with a single crack and the MoS_2 actuator were first relaxed for 50–200 ps at 4.2K within the NVT (fixed number of atoms N, volume V, and temperature T) ensemble. Non-periodic boundary conditions were applied in all three directions. After the relaxation, the strains were applied by displacing both ends at a uniform rate.

List of videos

Legend: FEM = Finite Element Method (The color map shows the normalized sum of the principal stresses, $w\sigma^p_{ii}/(Eh)$); MD = Molecular Dynamics; EXP = Experiments.

1. Single cut
   - **Single Cut FEM:** c7sm01693j10.mov
   - **Single Cut MD:** c7sm01693j11.mov
2. Pitch and lift modes combined
   - **Pitch Lift FEM:** c7sm01693j4.mov
   - **Pitch Lift EXP:** c7sm01693j3.mov
3. Lift mode (z–axis displacement)
   - **Lift FEM:** c7sm01693j2.mov
   - **Lift EXP:** c7sm01693j1.mov
4. Roll mode (rotation about x–axis)
   - **Roll, x–rotation FEM:** c7sm01693j9.mov
   - **Roll, x–rotation EXP:** c7sm01693j8.mov
5. Pitch mode (rotation about y–axis)
   - **Pitch, y–rotation FEM:** c7sm01693j6.mov
   - **Pitch, y–rotation EXP:** c7sm01693j5.mov
   - **Pitch, y–rotation MD:** c7sm01693j7.mov

6. Yaw mode (rotation about z–axis)
    - **Yaw, z–rotation FEM:** c7sm01693j13.mov
    - **Yaw, z–rotation EXP:** c7sm01693j14.mov

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