

## CURVED FOLDS ON SUPPORTED GRAPHENE UNDER COMPRESSION

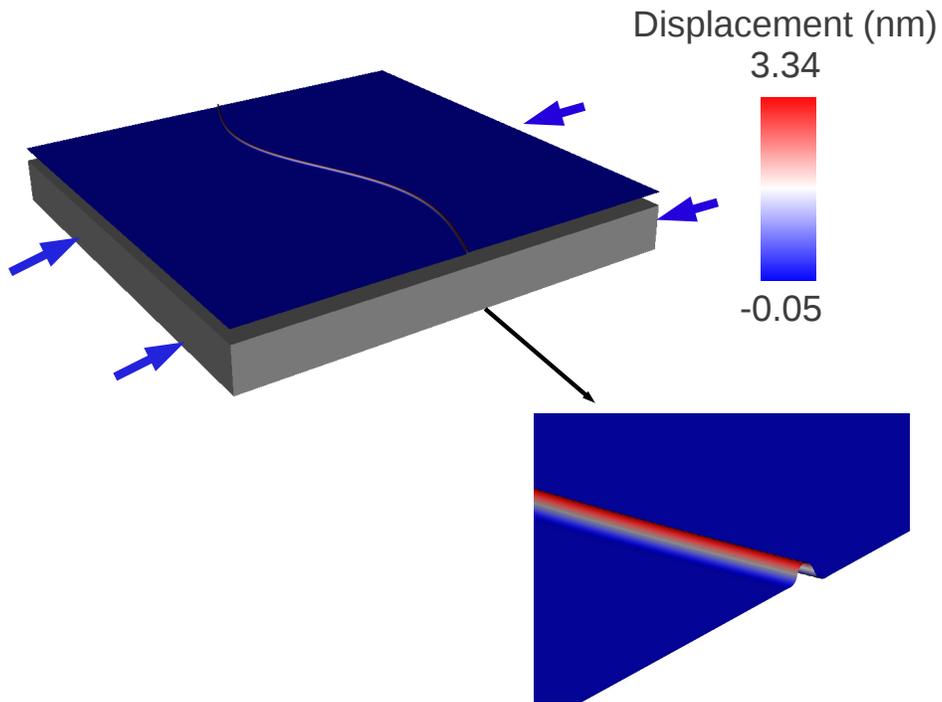
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Graphene, a flat monolayer of carbon atoms is a material of great interest due to its exceptional physical, chemical and electronic properties[1]. While in some cases graphene is freestanding, most often it is adhered to a substrate (supported graphene). As it is an extremely thin material graphene is very flexible and it is easily susceptible to out-of-plane buckling deformations. Graphene made by the process of chemical vapor deposition on metallic substrates like Cu or Ni exhibit a network of folds which delaminate from the substrate. This is due to the difference in the thermal expansion coefficients between graphene and the substrate, which creates a compressive strain on graphene on cooling. Such localized out-of-plane deformations, in the form of ridges or folds, strongly affect the electronic structure and the electronic, optical, or chemical properties of pristine graphene are modified, as shown experimentally [2, 3]. This may lead to failure of a device, or to tunable properties and new functionality if properly controlled. A very recent area of research is the strain-based engineering of graphene, exploiting the strong dependence of electronic properties of graphene and strain.

We systematically analyze the out-of-plane deformation of supported and laterally strained graphene by high-fidelity simulations based on an atomic-based continuum model [4]. We identify a strategy to control the fold network topology by forming patterns of weak adhesion on the substrate and by anisotropy of strain. It is found that the fold network follows the prescribed pattern on the substrate under certain conditions. Curved folds are formed on graphene by patterning the substrate of weak adhesion along a sinusoidal curve. While for lower curvatures of pattern the folds are stable with increasing strain, for higher curvatures the folds fragment after a certain strain to release the increasing stretching energy due to the curvature. Controlling the fold pattern can open pathways for novel applications in nanoelectromechanical devices. These curved folds could be exploited in graphene plasmonics to converge electromagnetic waves to increase the energy at the desired region.



**Figure 1:** A typical cross-section of a curved fold in graphene (blue) on a substrate (grey)

## REFERENCES

- [1] J. C. Meyer, A. K. Geim, M. I. Katsnelson, K. S. Novoselov, T. J. Booth, and S. Roth, The structure of suspended graphene sheets, *Nature*, 446, 60 (2007).
- [2] F. Guinea, B. Horovitz, and P. L. Doussal, Gauge field induced by ripples in graphene, *Physical Review B*, 77, 205421 (2008)
- [3] Wenjuan Zhu, Tony Low, Vasili Perebeinos, Ageeth A. Bol, Yu Zhu, Hugen Yan, Jerry Tersoff, and Phaedon Avouris. Structure and Electronic Transport in Graphene Wrinkles. *Nano Letters* 12 (7), 3431-3436, (2012)
- [4] Marino Arroyo and Ted Belytschko. An atomistic-based finite deformation membrane for single layer crystalline films. *Journal of the Mechanics and Physics of Solids*, 50(9):1941- 1977, (2002).
- [5] K. Zhang and M. Arroyo. Adhesion and friction control localized folding in supported graphene. *Journal of Applied Physics*, 113(19):193501, (2013)