Nov 03, 2017

The Shape, Energy, and Stability of Graphene Möbius Bands

Eliot Fried

Professor
Mathematics, Mechanics and Materials Unit,
Okinawa Institute of Science and Technology,
Okinawa, Japan

ABSTRACT:

Graphene is an extremely strong two-dimensional material but can easily bend, roll, and fold. This flexibility allows for the design complex three-dimensional nanostructures such as self-folding nanocages, which can be made utilizing origami and kirigami patterning. The Möbius band, a non-orientable one-sided surface constructed by twisting a rectangular strip about its long axis by 180 degrees and joining its short ends, is also a theoretically possible graphene-based nanostructure. Although a graphene Möbius band may simply be thought of a narrow ring with a half-twist, such objects have not yet been observed in the laboratory. In our molecular dynamics study, we obtain the equilibrium shapes and energies of armchair and zigzag edged Möbius bands made of various nanoribbon sizes in the zero temperature limit. Our simulation results show that graphene Möbius bands are mechanically stable and that, in spite of the discrete nature of the honeycomb lattice structure and associated edge types, their shapes surprisingly resemble those of continuum Möbius bands. We also find that the energy of a graphene Möbius band scales with the inverse of the length-to-width aspect ratio of the nanoribbon from which it is made. Furthermore, we demonstrate the effect of the presence of multiple twists and a buckling instability that arises above a certain threshold of twist.

BIOGRAPHY:

Eliot Fried obtained his Ph.D. in Applied Mechanics from the California Institute of Technology in 1991. He received a National Science Foundation Mathematical Sciences Postdoctoral Fellowship, a Japan Society for the Promotion of Science Postdoctoral Research Fellowship, and a National Science Foundation Research Initiation Award. Currently he is a Professor at the Okinawa Institute of Science and Technology Graduate University, where he leads the Mathematics, Mechanics, and Materials Unit. Previously, at McGill University, he was a Professor of Mechanical Engineering and the Tier 1 Canada Research Chair in Interfacial and Defect Mechanics. Before that he held tenured positions in the Department of Theoretical and Applied Mechanics at the University of Illinois at Urbana-Champaign and the Department of Mechanical and Aerospace Engineering at Washington University in St. Louis. At Illinois, he was a Fellow of the Center of Advanced Study and was awarded a Critical Research Initiative Grant. In his research, he uses statistical and continuum mechanics and thermodynamics, geometry, asymptotic analysis, bifurcation theory, and large-scale scientific computing to study both fundamental and applied problems involving novel material systems and processes.