

Collaborating teams apply findings developed at macroscale to materials at atomistic scale

PROBLEM

Graphene, discovered in 2004, is the thinnest known material. Because of its unique geometry — a single-atom thickness — fundamental questions about its mechanical performance remain unknown. A research team carried out a combined computational, theoretical and experimental study to see if an understanding of materials at the macroscale could be applied across the continuum to graphene.

MIT Professor Pedro Reis and co-authors wrote a series of papers explaining that the triangular-shaped tears that occur when a thin film is detached from a substrate are a signature mechanical behavior arising from the interaction of the three types of energy in the system: elasticity, adhesive energy and fracture energy. As the tape is pulled, the bending energy in the fold is converted into the surface energy of fracture and adhesion. Graphene inventor Kostya Novoselov, a fellow at the University of Manchester, had observed similar shaped tears at the nanoscale; when two-dimensional layers of graphene are scraped off graphite, they have a characteristic triangular shape. The researchers wondered if the analogous geometric shape of these materials indicates that the mechanical behavior is controlled by the same mechanisms.

APPROACH

MIT Professor Markus Buehler, who uses molecular dynamics simulation to explore the mechanical behavior of materials

at the nanoscale, and graduate student Dipanjan Sen worked with Reis and Novoselov to carry out atomistic-level simulations on graphene ribbons adhered to a substrate. Buehler's atomistic modeling is based on known chemical principles derived directly from quantum mechanics, and simulates the interactions of molecules under prescribed conditions, without the need to introduce empirical fitting parameters. It thus represents accurately the behavior of materials at the molecular level.

FINDINGS

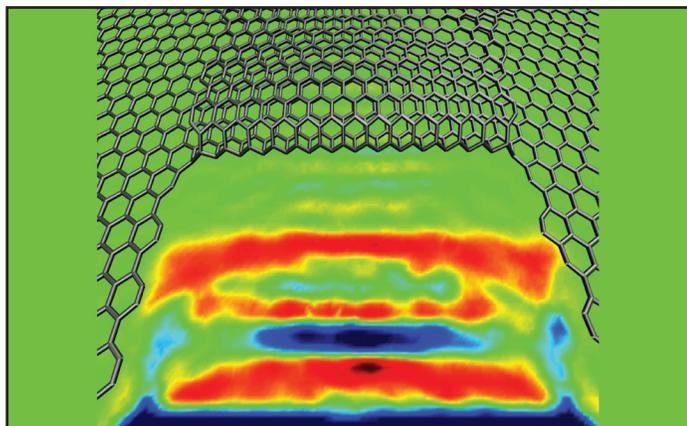
The team's atomistic simulations on graphene did not agree entirely with the existing model describing a materials' behavior at the macroscale. After careful deliberation on the problem, Sen recognized that the contributor to elasticity in a macroscale system — the bending energy — was minimal at the atomic scale. At the macroscale, bending energy is a combination of stretching (on the top side of the material) and compression (on the bottom), and scales as the cube of the thickness of the material. But a two-dimensional material like graphene has no thickness, and bending energy arises only from changes in the bonds and angles between atoms. The researchers found that at the nanoscale, the bending energy can be ignored in favor of the stretching energy stored in the sheet, which is concentrated in a roughly elliptical region of the sheet just ahead of the fold and in the stretching of the torn ribbon. These numerical results are in excellent agreement with the tapered ribbons Novoselov obtained by tearing graphene sheets in nanoscale experiments.

IMPACT

This work demonstrates how an understanding of materials at the macroscale can be applied with modifications to materials at the nanoscale. The findings also define a significant aspect of the mechanical behavior of graphene that could lead to improved manufacturing techniques for this material, which has exceptional properties that many researchers believe will lead to the next generation of electronics or composite materials. Of particular significance is the fact that graphene's conductivity alters with the width of the ribbon. The ability to control the tearing angle has the potential to transform the way graphene strips are used.

MORE

This work was published in the May 21 issue of *Small*.



A two-dimensional graphene sheet being pulled from an adhesive substrate will form triangular shaped ribbons. Graphic / Dipanjan Sen

