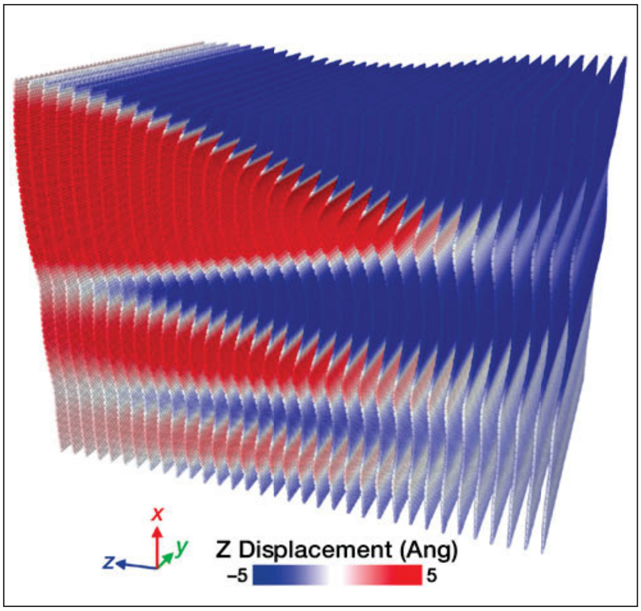
## Ripplocation deformation mechanism describes buckling and kinking of bulk layered materials

Layered materials are encountered almost daily: pencils, clays, and ice cubes are the most common examples of this diverse family of solid materials. They include naturally and artificially synthesized structures and increasingly find more complex uses in biosensors, batteries, and nuclear reactors. The crystal structure of layered materials confines deformation—like a deck of cards—to two dimensions. Consequently, the deformation mode is unique: the layers form kink bands, and the solids exhibit reversible stress–strain loops during compression. Although researchers have proposed basal dislocations and bowing of dislocations as possible operative plastic deformation mechanisms, these are still disputed and cannot fully explain the kinking nonlinear elastic behavior or *c*-axis strain of many layered materials. Dislocations are the defects responsible for plastic deformation in the vast majority of metallic materials.

Researchers have now proposed a new fundamental micromechanism—a ripplocation—to explain the deformation of layered materials. The term "ripplocation" was coined by Akihiro Kushima and colleagues in early 2015 to describe the buckling of a surface or near surface layer in van der Waals two-dimensional solids (*Nano Letters*, doi:10.1021/nl5045082). The work by several research groups at Drexel University expanded the understanding of this mechanism. Professors Michel W. Barsoum, Garritt J. Tucker, and Mitra L. Taheri, along with their students—Jacob Gruber, Andrew C. Lang, and Justin Griggs—relied on computational modeling and transmission electron microscope (TEM) imaging to make the case that ripplocations are the operative mechanism in the deformation of layered solids. They published their results in a recent issue of *Scientific Reports* (doi:10.1038/srep33451).

Barsoum says, "I have been working on the deformation of layered solids for almost two decades and I tried to explain their deformation in terms of basal dislocations; it was not working too well. When I read the paper by Kushima et al., I immediately realized the full implications of their work; that it was not just applicable to van der Waals solids, but was a fundamental mechanism underlying the deformation of all layered solids."




The schematic shows the displacement of graphitic atomic planes to the left (red) and right (blue) as a cylindrical indenter (50-nm diameter) is pushed into the surface from the top. The image shows approximately three kink bands. Credit: Garritt J. Tucker.

The researchers modeled the kinking behavior on graphite and simulated surface and bulk ripplocations in constrained (non-deformed, immovable adjacent layers) and unconstrained (nearby layers that are free to buckle) systems. Under in-plane strain, the materials deformed until buckles, folds, and kinks nucleated in order to reduce the total energy of the system. The constraint of the bulk systems significantly affected both the size of the folds and depended on the energy required to deform the surrounding lattice. The researchers effectively used their computational analysis of ripplocations to describe the deformation of graphite. They further showed that ripplocations—unlike dislocations—have no Burgers vector and no polarities.

To observe bulk ripplocations experimentally, the researchers relied on $Ti_3SiC_2$, a layered transition-metal carbide (which are commonly known as MAX phases), and used nano-indentation to induce kinking in the layers below the indenter. Analysis of transmission electron microscopy images showed evidence for *c*-lattice strain eliminating the possibility that the observed distortions could have originated from basal dislocations. Based on these results and the fact that the indentation-induced damage and pileup of material at the edges of the indentation mark, it was concluded that bulk ripplocations were the main deformation drivers.

The ripplocation mechanism helps explain several observations in the deformation and stress–strain behavior of layered materials that to date have been unexplained, not the least of which is kink band formation, a ubiquitous feature characteristic of the deformation of all layered solids, from geologic formations to card decks. This recent effort further expanded the understanding of this concept and included kinking behaviors inside of bulk structures. Layered and two-dimensional materials, which exhibit promising mechanical, optical, and electronic properties, have attracted significant interest. Fundamental insight into their unique deformation behavior will improve understanding of their stress mitigation, delamination, and interaction with point defects. These findings, in turn, are crucial for subsequent design of devices and composites that may implement this large family of materials.

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