BOROPHENE

Served on a silver platter

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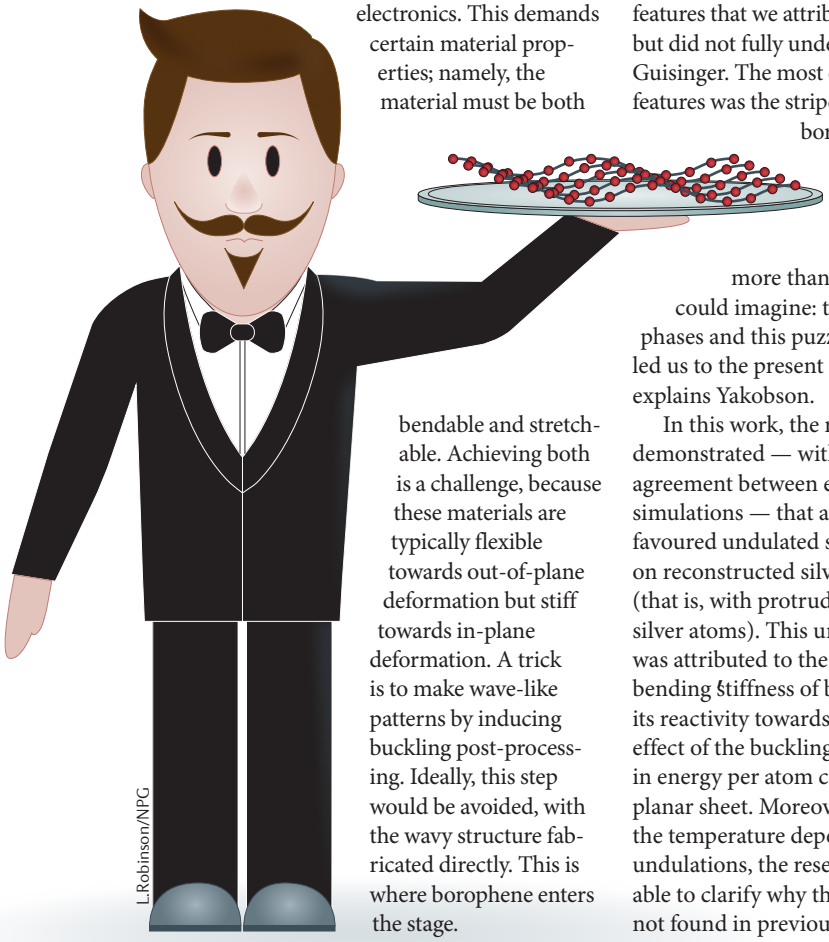
When the 2D allotrope of boron — borophene — was first synthesized in late 2015, it displayed curious features not observed in other 2D materials, including a striped pattern. Now, combining first-principles calculations with ultrahigh vacuum scanning tunnelling microscopy, this pattern is revealed as energetically favoured undulations. This study, reported in *Nano Letters*, expands our knowledge of this new 2D material and has implications for the development of flexible and wearable electronic devices.

One of the many areas of interest for 2D materials is in flexible electronics. This demands certain material properties; namely, the material must be both bendable and stretchable. Achieving both is a challenge, because these materials are typically flexible towards out-of-plane deformation but stiff towards in-plane deformation. A trick is to make wave-like patterns by inducing buckling post-processing. Ideally, this step would be avoided, with the wavy structure fabricated directly. This is where borophene enters the stage.



L.Robinson/NPG

Borophene was first predicted by Boris Yakobson, Rice University, who co-led the present study. "We predicted a variety of boron polymorphs and then even suggested which exactly should form on a 'silver platter'. This culminated when the Northwestern and Argonne guys produced it in the lab!", says Yakobson. The two groups he refers to are those of Mark Hersam and Nathan Guisinger, who teamed up with Yakobson in this work. "Guided by predictive modelling, we recently discovered and experimentally synthesized a new 2D boron allotrope. Our atomic-scale characterization revealed several interesting features that we attributed to strain but did not fully understand," says Guisinger. The most exciting of these features was the striped pattern that borophene assumed on a silver substrate. "The experiment showed more than we theorists could imagine: these striped phases and this puzzling pattern led us to the present collaboration," explains Yakobson.

In this work, the researchers demonstrated — with excellent agreement between experiment and simulations — that an energetically favoured undulated structure forms on reconstructed silver substrates (that is, with protruding rows of silver atoms). This unique behaviour was attributed to the very small bending stiffness of borophene and its reactivity towards silver. The net effect of the buckling is a reduction in energy per atom compared with a planar sheet. Moreover, by studying the temperature dependence of undulations, the researchers were able to clarify why this structure was not found in previous studies where borophene was synthesized at a lower temperature.

The undulated structure is likely to confer high stretchability and compressibility if the borophene were transferred to an elastomeric substrate. In addition, the electrical properties are robust towards the undulated pattern, which is essential for realizing flexible electronic devices. A remaining challenge lies in removing the borophene from the silver substrate; however, the researchers suggest that recently developed transfer methods could be applied to preserve the structure. The next steps include "determining the atomic structure of other phases of borophene, performing further property characterization, and ultimately developing applications (such as flexible and stretchable electronics) for this new material," says Hersam. On a theoretical level, the goals will be "to understand the kinetics of growth and how and why it leads to different morphologies; to explore and model possible plasmonic behaviours; and to look more carefully into Dirac cones in the electronic band structure," adds Yakobson.

Tangential to the new insight provided, this work is a pertinent example of the importance of computational methods for materials discovery: "To advance this field, it is imperative that a strong synergy between theory and experiment persists," concludes Guisinger.

Adam Brotchie

ORIGINAL ARTICLE Zhang, Z. *et al.* Substrate-induced nanoscale undulations of borophene on silver. *Nano Lett.* http://dx.doi.org/10.1021/acs.nanolett.6b03349 (2016)

FURTHER READING Mannix, A. J. *et al.* Synthesis of borophenes: anisotropic, two-dimensional boron polymorphs. *Science* **350**, 1513–1516 (2015) | Liu, Y, Penev, E. S. & Yakobson, B. I. Probing the synthesis of two-dimensional boron by first-principles computations. *Angew. Chem. Int. Ed.* **52,** 3156–3159 (2013)