Study explores mechanical properties of molybdenum disulfide nanoribbons with armchair edges

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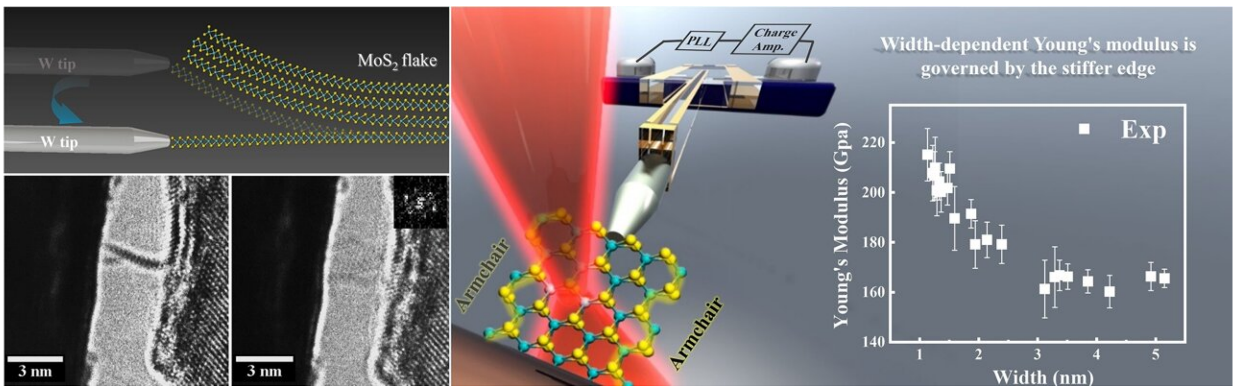

Mechanical properties of single-layer MoS_2 nanoribbons investigated using a new micromechanical measurement method. Image Caption: (Upper left) Illustration showing the process of contacting a tungsten (W) tip to the edge of MoS_2 multilayer and peeling off the outermost single-layer MoS_2 nanoribbon. (Lower left) TEM image of the single-layer MoS_2 nanoribbon observed from the cross-section and from the plane. (Middle) schematic illustration of the in situ TEM experiment on the nanoribbon with armchair edges, and (right) Young's modulus of the nanoribbon as a function of its width. Credit: Yoshifumi Oshima from JAIST

The properties of nanoribbon edges are important for their applications in electronic devices, sensors, and catalysts. A group of scientists from Japan and China studied the mechanical response of single-layer molybdenum disulfide nanoribbons with armchair edges using in situ transmission electron microscopy.

They showed that the nanoribbon Young's modulus varied inversely with its width below the width of 3nm, indicating a higher bond stiffness for the armchair edges. Their work, published in the journal *Advanced Science*, was co-authored by Associate Professor Kenta Hongo and Professor Ryo Maezono from JAIST and Lecturer Chunmeng Liu and Lecturer Jiaqi Zhang from Zhengzhou University, China.

Sensors have become ubiquitous in the modern world, with applications ranging from detecting explosives, measuring physiological spikes of glucose or cortisol non-invasively to estimating greenhouse gas levels in the atmosphere.

The primary technology required for sensors is a mechanical resonator. Traditionally, quartz crystals have been used for this purpose owing to their high rigidity and easy availability. However, this technology has recently given way to advanced nanomaterials. One such promising material is the single-walled molybdenum disulfide (MoS_2) nanoribbon.

Characterizing the physical and chemical properties of nanoribbon edges is crucial for their applications in electronic devices, sensors, and catalysts. However, the mechanical response of MoS_2 nanoribbons—expected to be dependent on their edge structure—has remained unexplored, hindering their practical implementation in thin resonators.

Against this background, a group of scientists from Japan and China, led by Professor Yoshifumi Oshima from Japan Advanced Institute of Science and Technology (JAIST), investigated the mechanical properties—namely the Young's modulus—of single-layer MoS_2 nanoribbons with armchair edges as a function of their width using a micromechanical measurement method.

Prof. Oshima says, "We have developed the world's first micromechanical measurement method to clarify the relationship between the atomic arrangement of atomic-scale materials and their mechanical strength by incorporating a quartz-based length extension resonator (LER) in an in situ transmission electron microscopy (TEM) holder."

Since the resonance frequency of a quartz resonator changes when it senses contact with a material, the equivalent spring constant of the material can be estimated with high precision by the change in this resonance frequency. Moreover, it is possible to capture high-resolution TEM images as the LER vibration amplitude necessary for the measurement is as small as 27 pm. Consequently, the novel method developed by the researchers managed to overcome the shortcomings of conventional techniques, achieving high-precision measurements.

The researchers first synthesized a single-layer MoS_2 nanoribbon by peeling off the outermost layer of the folded edge of an MoS_2 multilayer using a tungsten tip. The single-layer nanoribbon was supported between the multilayer and the tip.

The TEM image of this MoS_2 nanoribbon revealed that its edge had an armchair structure. "The width and length of the nanoribbon were also measured from the image, and the corresponding equivalent spring constant was determined from the frequency shift of the LER to obtain the Young's modulus of this nanoribbon," said Lecturer Chunmeng Liu.

The researchers found that the Young' modulus of the single-layer MoS_2 nanoribbons with armchair edges was dependent on their width. While it remained constant around 166 GPa for wider ribbons, it showed an inverse relation to the width for ribbons below 3nm in width, increasing from 179 GPa to 215 GPa as the nanoribbon width decreased from 2.4nm to 1.1nm. The researchers attributed this to a higher bond stiffness for the edges compared to that of the interior.

Density functional theory calculations performed by the researchers for explaining their observation revealed that the Mo atoms buckled at the armchair edge, which resulted in electron transfer to the S atoms on both sides. This, in turn, increased the Coulombic attraction between the two atoms, enhancing the edge strength.

This study sheds important light on the mechanical properties of MoS_2 nanoribbons, which could facilitate the design of nanoscale, ultra-thin mechanical resonators.

"Nanosensors based on such resonators can be integrated into smartphones and watches, which will enable people to monitor their environment as well as communicate the sense of taste and smell in the form of numerical values," concludes Lecturer Jiaqi Zhang.

More information: Chunmeng Liu et al, Stiffer Bonding of Armchair Edge in Single-Layer Molybdenum Disulfide Nanoribbons, *Advanced Science* (2023). DOI: 10.1002/advs.202303477

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