Review of recent advances in the mechanics of two-dimensional materials

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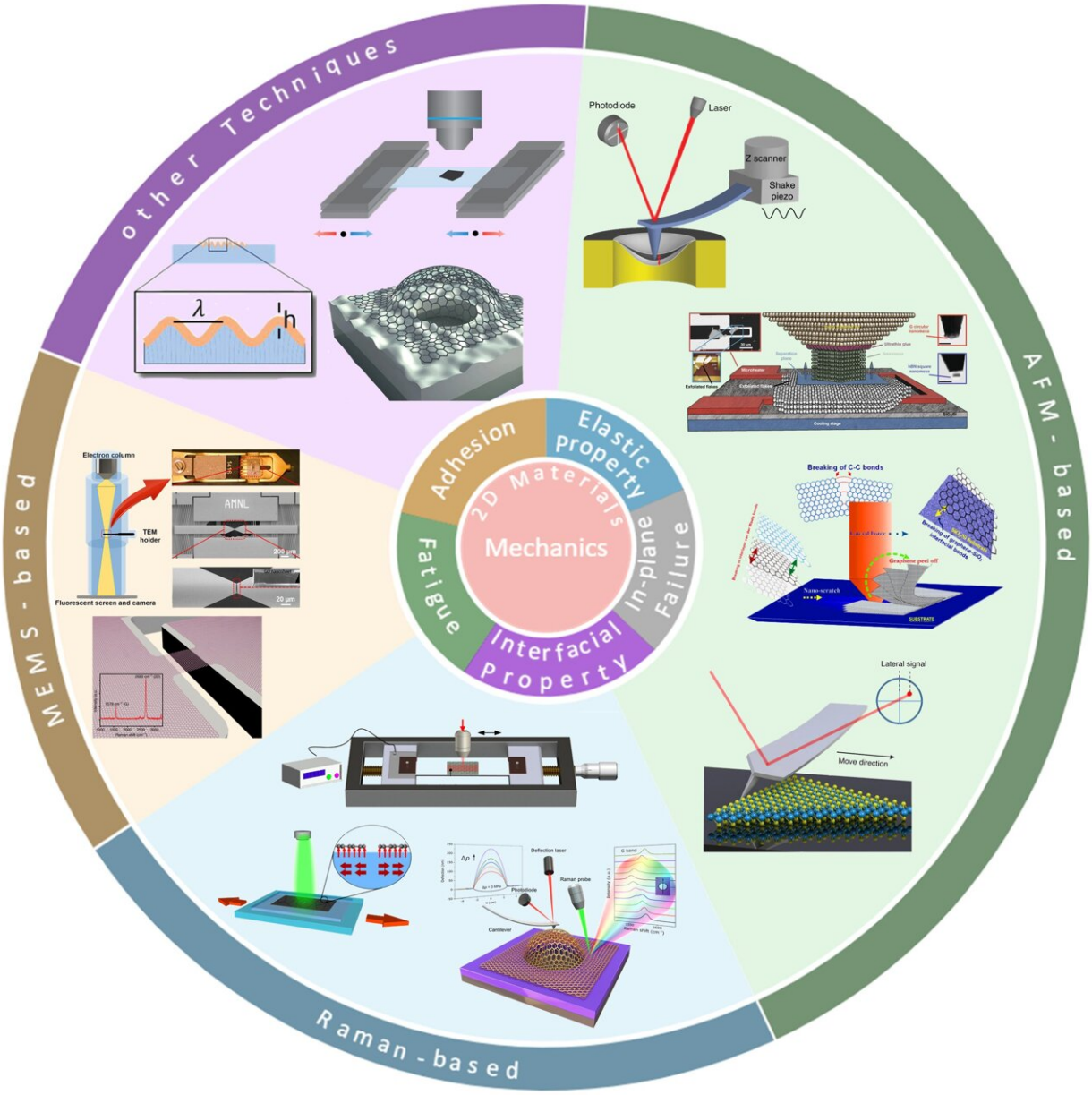

In this article, the recent discoveries in the field of the mechanics of 2D materials are reviewed, including mechanical properties recently characterized (e.g., elastic, fracture, adhesion, friction, and fatigue), novel deformation mechanisms, state-of-the-art characterization technologies, and advancement in computational technologies. Credit: Guorui Wang, Hongyu Hou, Yunfeng Yan, Ritesh Jagatramka, Amir Shirsalimian, Yafei Wang, Binzhao Li, Matthew Daly and Changhong Cao

Publishing in the *International Journal of Extreme Manufacturing*, scientists from McGill University, University of Illinois, and University of Science and Technology of China comprehensively reviewed the most recent discoveries in the field of the mechanics of 2D materials by discussing various key mechanical properties, including the elastic properties, in-plane failure, fatigue, interfacial shear/friction, and adhesion. Four main aspects were focused: recent discoveries in the mechanical properties, novel deformation mechanisms, characterization technologies, and computational advancement.

The leading team principal investigator, Prof. Changhong Cao, commented, "by reviewing the intrinsic and extrinsic factors that govern 2D material mechanics, we hope that the community may draw design strategies for structural and interfacial engineering of 2D material systems for novel applications."

While substantial efforts have been made recently in the experimental investigation of the mechanical properties of 2D materials through various techniques as reviewed in the article, current research on the mechanics of 2D materials beyond graphene is still in its nascent stage, especially for emerging 2D materials such as metal-organic frameworks (MOFs) and covalent organic frameworks (COFs).

The first author, Prof. Guorui Wang said, "In addition to COFs and

MOFs, we found that while a number of transition-metal dichalcogenides (TMDs), such as MoS_2, WS_2, $MoSe_2$, and WSe_2, have been widely studied, few mechanical investigations have been performed on other TMDs (e.g., VS_2, $MoTe_2$, $TaSe_2$, etc.), as well as TMD alloys which exhibit unique chemical, electronic and magnetic properties."

In addition, while 2D heterostructures can be designed and built either by manual- or self-assembly techniques in vertical or lateral fashions, there is, however, a dearth of information concerning the mechanical behaviors of 2D heterostructures.

The co-first author, Hongyu Hou, a doctoral candidate at McGill, added that "currently, most mechanical studies of 2D materials focus on the static or quasi-static performance, while the dynamic behaviors in response to cyclic loading or impact loading are largely unexplored."

Moreover, the practical challenges in the handling and experimental testing of ultrathin systems reinforce the value of accurate computational methodologies to screen the vast mechanical property space of 2D materials.

An expert in computational mechanics and also the co-leading author of the article, Prof. Matthew Daly, commented, "with respect to the computational mechanics studies of 2D materials, there are also numerous advancement and future opportunities. For example, while DFT simulations offer a pathway to study the mechanics of these systems using first-principles approaches, the high computational cost and limitations on simulation size limit the application of this method to complex 2D systems (e.g., multilayers and heterostructures)."

"MD-based simulations greatly increase the accessible length-scales but present their own challenges in the limited availability of interatomic potentials for 2D materials. Machine learning presents a new opportunity

to create interatomic potentials for 2D systems without the need to develop deep domain expertise in each system of interest. In addition, strain engineering of functional properties presents an inevitable next-step in the study of 2D materials. Despite some early progress in strain engineering topics, non-trivial challenges remain."

More information: Guorui Wang et al, Recent advances in the mechanics of 2D materials, *International Journal of Extreme Manufacturing* (2023). DOI: 10.1088/2631-7990/accda2