

Scientists develop new system to record 2D crystal synthesis in real time

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False-color optical image of the MoS2 crystals grown at a high temperature and low flow rate, where the largest average crystal size is obtained among the tested growth conditions. Credit: Jun Lou/Rice University

Materials scientists at Rice University are shedding light on the intricate growth processes of 2D crystals, paving the way for controlled synthesis of these materials with unprecedented precision.



Two-dimensional materials such as graphene and <u>molybdenum disulfide</u> (MoS_2) exhibit unique properties that hold immense promise for applications in electronics, sensors, energy storage, biomedicine and more. However, their complex growth mechanisms—inconsistent correlations exist between how the conditions for growth affect the shapes of crystals—have posed a significant challenge for researchers.

A research team at Rice's George R. Brown School of Engineering tackled this challenge by developing a custom-built miniaturized chemical vapor deposition (CVD) system capable of observing and recording the growth of 2D MoS₂ crystals in real time. The work is published online in the journal *Nano Letters*.

Through the use of advanced image processing and machine learning algorithms, the researchers were able to extract valuable insights from the <u>real-time</u> footage, including the ability to predict the conditions needed to grow very large, single-layer MoS_2 crystals.

Study co-author Jun Lou, professor and associate chair of the Department of Materials Science and Nanoengineering at Rice, said this <u>interdisciplinary approach</u> represents a significant step forward in the field of scalable synthesis of 2D materials.

"By combining real-time experimental observations with cutting-edge machine learning techniques, we have demonstrated the potential to predict and control the growth of 2D crystals with excellent accuracy," Lou said.

The research team's findings have far-reaching implications for the future of 2D materials. Driven by their success with MoS_2 , the researchers believe that their approach can be extended to other 2D materials and heterostructures, offering a powerful platform for designing and engineering next-generation 2D materials with tailored



properties.

"For example, in electronics, being able to robustly synthesize 2D crystals like MoS_2 at scale could lead to faster and more efficient devices," Lou said. "In sensors, it could lead to more sensitive and selective devices."

"This research is an important step toward realizing the full potential of 2D materials and paves the way for the development of innovative technologies that could revolutionize a wide range of industries," said Ming Tang, associate professor of materials science and nanoengineering and study co-author.

Joining Lou and Tang on the study from the Rice Department of Materials Science and Nanoengineering are Jing Zhang, Tianshu Zhai, Faizal Arifurrahman, Yuguo Wang, Andrew Hitt, Zelai He, Qing Ai, Yifeng Liu, Chen-Yang Lin and Yifan Zhu.

More information: Jing Zhang et al, Toward Controlled Synthesis of 2D Crystals by CVD: Learning from the Real-Time Crystal Morphology Evolutions, *Nano Letters* (2024). DOI: 10.1021/acs.nanolett.3c04016

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