UC Irvine researchers discover atomic-level mechanism in polycrystalline materials

Findings could herald more efficient electronics, aerospace and automotive technologies.
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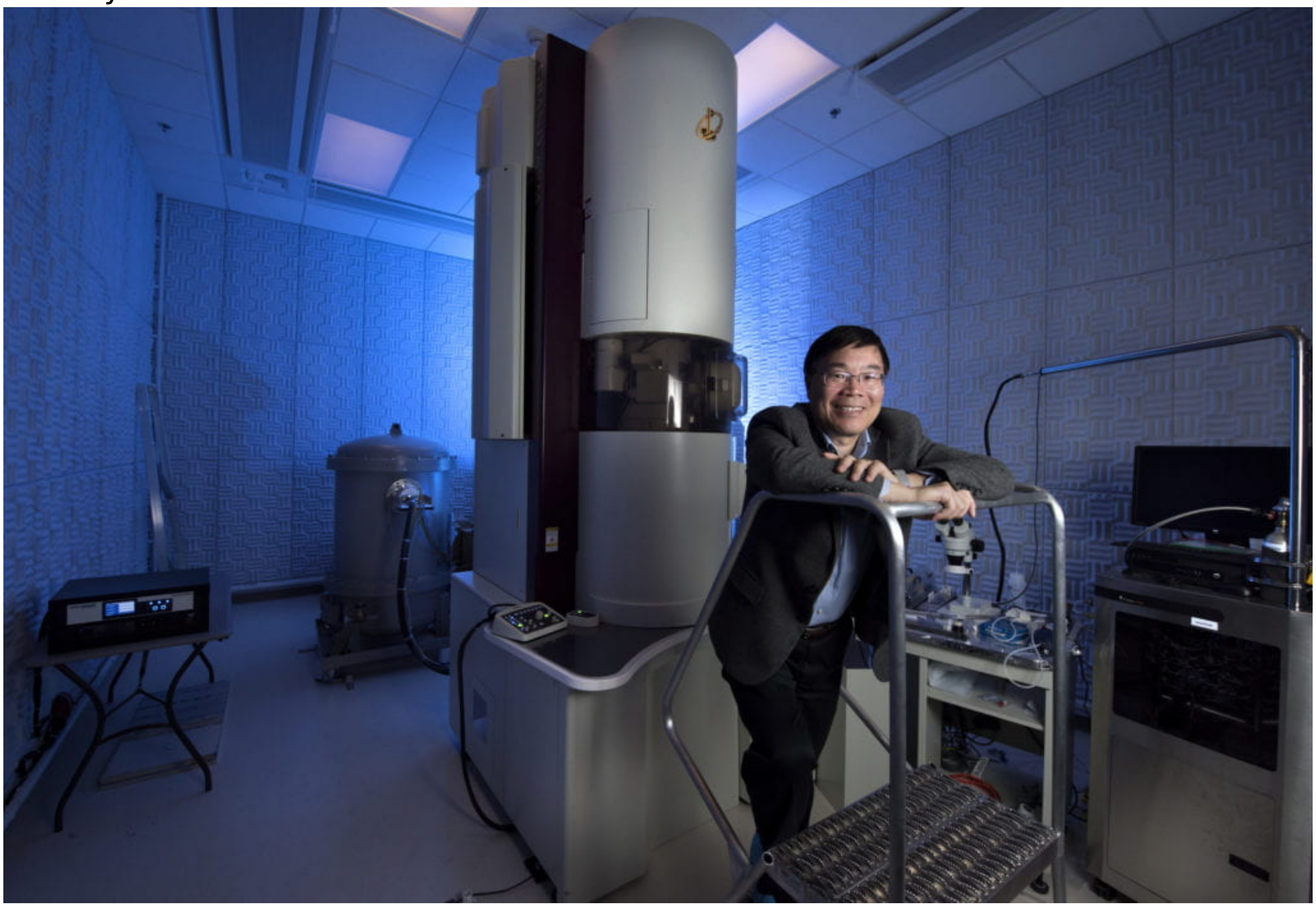

“Scientists have speculated and theorized on phenomena occurring at the boundaries of crystalline grains for decades, but now – through the use of the most advanced instruments available to the scientific community – we have been able to transition from theory to observation,” says Xiaoqing Pan, UC Irvine Distinguished

Professor of materials science and engineering and director of the UC Irvine Materials Research Institute. He's lead author of a paper in Science on direct observations of grain rotation in polycrystalline materials.

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Irvine, Calif., Oct. 8, 2024 — Researchers at the University of California, Irvine and other international institutions have for the first time achieved atomic-scale observations of grain rotation in polycrystalline materials. Widely used in electronic devices, aerospace technologies, automotive applications and solar energy systems, these substances have long been studied for their unique properties and structural dynamics.

Using state-of-the-art microscopy tools housed in the UC Irvine Materials Research Institute, scientists were able to heat samples of platinum nanocrystalline thin films and observe the mechanism driving grain rotation in unprecedented detail. Their findings are the subject of a paper published recently in *Science*.

The study employed advanced techniques such as four-dimensional scanning transmission electron microscopy and high-angle annular dark-field STEM. To address the challenge of interpreting the large 4D-STEM datasets, the authors developed a novel machine learning-based algorithm to extract critical information from the data. These powerful imaging and analysis tools provided direct, real-time views of the atomic processes involved, specifically highlighting the role of disconnections at grain boundaries.

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Grain boundaries, the interfaces between individual crystal grains in polycrystalline materials, are known to harbor imperfections that can impact conductivity and efficiency. The researchers discovered that grain rotation in these substances occurs through the propagation of disconnections – line defects with both step and dislocation characteristics – along the grain boundaries. This insight significantly advances understanding of the microstructural evolution in nanocrystalline materials.

With the machine learning-assisted data analysis, the study also revealed for the first time a statistical correlation between grain rotation and grain growth or shrinkage. This relationship arises from shear-coupled grain boundary migration driven by disconnection motion, as confirmed by STEM observations and supported by atomistic simulations. This finding is pivotal as it not only illuminates the fundamental mechanisms of grain rotation but also offers insights into the dynamics of nanocrystalline materials.

“Our results provide unequivocal, quantitative and predictive evidence of the mechanism by which grains rotate in polycrystals on an atomic scale,” said Pan, who is also a professor in UC Irvine’s Department of Physics & Astronomy, a Henry Samueli Endowed Chair in Engineering, and director of the UC Irvine Center for Complex and Active Materials. “Understanding how disconnections control grain rotation and grain boundary migration processes can lead to new strategies for optimizing the microstructures of these materials. This knowledge is invaluable for advancing technologies in various industries, including electronics, aerospace and automotive sectors.”

The research offers fresh prospects for improving the performance and reliability of polycrystalline materials, making them more efficient and durable for a wide range of applications.

Pan’s collaborators on this project were Yutong Bi, Ying Han, Yuan Tian and Mingjie Xu of UC Irvine; Xiaoguo Gong and David Srolovitz of the University of Hong Kong; Leonardo Velasco Estrada of Colombia National University; Evgeniy Boltynjuk of Germany’s Karlsruhe Institute of Technology; Horst Hahn of the University of Oklahoma; and Caihao Qiu and Jian Han of City University of Hong Kong. The research was supported by the National Science Foundation’s Materials Research Science and Engineering Centers program, the U.S. Army Research Office and the Hong Kong Research Grants Council.

About UC Irvine’s Brilliant Future campaign: Publicly launched on Oct. 4, 2019, the Brilliant Future campaign aims to raise awareness and support for UC Irvine. By engaging 75,000 alumni and garnering $2 billion in philanthropic investment, UC Irvine seeks to reach new heights of excellence in student success, health and wellness, research and more. The Henry Samueli School of Engineering plays a vital role in the success of the campaign. Learn more by visiting https://brilliantfuture.uci.edu/the-henry-samueli-school-of-engineering.

About the University of California, Irvine: Founded in 1965, UC Irvine is a member of the prestigious Association of American Universities and is ranked among the nation's top 10 public universities by *U.S. News & World Report*. The campus has produced five Nobel laureates and is known for its academic achievement, premier research, innovation and anteater mascot. Led by Chancellor Howard Gillman, UC Irvine has more than 36,000 students and offers 224 degree programs. It's located in one of the world's safest and most economically vibrant communities and is Orange County's second-largest employer, contributing $7 billion annually to the local economy and $8 billion statewide. For more on UC Irvine, visit www.uci.edu.

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