

# Integrating in situ experiment and atomistic modeling to decipher grain boundary deformation mechanisms

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With recent advances in atomistic modeling and in situ experimental technologies, there have been increased efforts to combine these approaches to understand the atomistic deformation mechanisms at grain boundaries (GBs). Here I will present our recent studies that integrate in situ electron microscopy, nanomechanical testing, and atomistic modeling to investigate GB deformation mechanisms. For example, we have combined in situ high resolution transmission electron microscopy experiments and atomistic simulations to unravel the atomic-scale processes of stress-driven GB sliding and structural transformation that occur unexpectedly at room temperature. We have also combined in situ MEMS-based nanomechanical testing and atomistic reaction pathway simulations to uncover the rate-controlling GB processes that dictate the experimentally measured activation volumes in nanocrystalline metals. The ability to resolve the atomic-scale dynamic processes of GB deformation, through coupled in situ experiment and atomistic modeling, enables a deep understanding of how GBs affect the plastic behavior of polycrystalline materials.



**Bio:** Ting Zhu is a Woodruff Professor in the Woodruff School of Mechanical Engineering at Georgia Institute of Technology. He received his Ph.D. in Mechanical Engineering from Massachusetts Institute of Technology in 2004. He worked as a postdoctoral associate at Harvard University before joining Georgia Tech in 2005. His research is focused on mechanics and materials modeling. He received the Sia Nemat-Nasser Early Career Award from the American Society of Mechanical Engineers and the Young Investigator Medal from the Society of Engineering Science. The Zhu group website is <https://www.zhugroup.gatech.edu/>.