# 北京大学工学院
# 力学与工程科学系学术报告

## Atomistic modeling of hydrogen impact on metals


**报告人：Shigenobu Ogata**

Osaka University, Japan


时　间：9 月 2 日（周一）15:00-16:30

地　点：新奥工学大楼 3F-3048 会议室

**报告摘要：**


The study of hydrogen's behavior and its impact on deformation and fracture in metals has been extensive, with numerous models and theories developed. However, direct observation of hydrogen in materials remains challenging, leaving many questions unanswered. Atomistic simulation emerges as a valuable tool for directly investigating hydrogen behaviors and their effects on deformation and fracture. The effectiveness of these simulations largely depends on accurately describing atomic interactions within the iron hydrogen system. Recent advancements include the proposal of artificial neural network (ANN) atomic interactions for the iron-hydrogen binary system, trained using a dataset based on Density Functional Theory (DFT) calculations of energy, force, and structure. These ANN atomic interactions combine the computational efficiency of empirical models with the accuracy and transferability of DFT, allowing for a quantitative elucidation of phenomena contributing to hydrogen embrittlement. This has led to a clearer understanding of how hydrogen influences vacancy movement, dislocation activities, and the mechanisms behind crack formation at both grain boundaries and within grains.


**报告人简介：**

Dr. Shigenobu Ogata is a Full Professor in the Department of Mechanical Science and Bioengineering in Osaka University. He is also Research Affiliate of the Department of Nuclear Science and Engineering, Massachusetts Institute of Technology (MIT), USA. He received his Ph.D. degree in Mechanical Engineering from Osaka University in 1998. He was a visiting research scientist in the Department of Nuclear Science and Engineering at MIT(USA) 2001 – 2002. He is an editor of Progress in Materials Science (IF: 37.400). He and his group aim to develop reliable theoretical models and neural network models for describing various nonlinear multiscale and/or multiphysics phenomena that appear in solid materials, and then to design materials with novel functions and a deformation process controlled at an atomic level in a predictive manner. He developed many mature and widely accepted models for the strength and deformation of materials: Amorphous deformation, Strength of crystal, Dislocation and Diffusion driven deformation, Hydrogen embrittlement and so on. He has published over 200 papers in Science, Advanced Materials, Nat. Commun., Nano Letters, Phys. Rev. B, Acta Mater. and other international journals that received 9500+ citations and 43 h-index (5100+ citations and 37 h-index since 2019). His awards more than 20 include: Lee Hsun Lecture Award of Institute of Metal Research, China (2014)

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